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Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns Section 16—Data for 86 Substances

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, it must be used in ordering. All are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 16. --- Data for 86 Substances

Ъу

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and

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Standard x-ray diffraction patterns are presented for 86 substances. Fifty-eight of these patterns represent experimental data and 28 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data , the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 86 compounds (58 experimental and 28 calculated patterns), and is the twentysixth of the series of "Standard X-ray Diffraction Powder Patterns "2,

EXPERIMENTAL POWDER PATTERNS

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts.

IJCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the samples improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of 20 were taken at positions about 20% of the way down from the top, and in the center of the peak width. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks were not reported.

At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for $K\alpha_1$ and were applied to the unresolved low angle peaks, as well as to the resolved $K\alpha$, peaks in the higher angle regions. If the internal standard correction varied along the length of the pattern, linear interpolations were used.

²See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 20 angles were computed using cell dimensions uncorrected for index of refraction.

Table 1

Calcu	ılated 2θ Angles,	$CuK\alpha_1 \lambda = 1$.540598Å
hkl	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088A ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 \pm 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: $\lambda \, (\text{CuK}\alpha_1, \, \text{peak}) = 1.540598 \text{\AA}$ [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order

to follow the convention of Crystal Data [1973].

A computer program [Evans et al., 1963] assigned hkl's and refined the lattice constants. Cell refinement was based only upon $2\theta_{\rm obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma (\theta_{\rm obs} - \theta_{\rm calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, multiple hkl's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest \underline{h} was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

<u>Densities</u>. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights published by the International Union of Pure and Applied Chemistry [1972].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \le 2$) [de Wolff, 1968]. All patterns reported in this publication have M_{20} between 20 and 233, and $X_{20} = 0$ unless noted otherwise. M_{20} was specified for any pattern indexed with a cell derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings is conveniently reported as FN [Smith and Snyder, 1979]. The format used in this publication was F_N = overall value ($\Delta 20$, N_{DOSS}), where N, the number of observed reflections was chosen as 30 or the maximum number of lines of the pattern, if the entire pattern had fewer than 30 lines. The "overall value" was the figure of merit, F_N, as defined by Smith and Snyder [1979], and $\Delta 20$ was the average absolute magnitude of discrepancy between observed and calculated 20 values for the N lines. $\rm N_{\hbox{\scriptsize poss}}$ was the number of unique and resolvable diffraction lines allowed in the space group, up to the Nth observed and indexed line. In this publication, the value of $F_{\rm N}$ ranged from 31 to 118, with an average value of 61 for the 58 patterns from experimental data.

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed,

a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position.



With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.



Reference Intensity Ratio, $I/I_{\rm corundum}$. The reference intensity ratio, $I/I_{\rm c}$, has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113 (hexagonal) of corundum (α -Al₂O₃) [Visser and de Wolff, 1964]. In this publication, the ratios $I/I_{\rm c}$ were tabulated for copper K α radiation, for a 1:1 mixture by weight of the sample and corundum. Occasionally $I/I_{\rm c}$ was not determined because it was not feasible.

A procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, $\mathbf{x_S}$ and $\mathbf{x_C}$ $(\mathbf{x_S}=1-\mathbf{x_C})$, the intensities for reflection $\underline{\mathbf{h}}$ of the sample and $\underline{\mathbf{k}}$ of corundum were measured for several combinations of $\underline{\mathbf{h}}$ and $\underline{\mathbf{k}}$ usually within the same region of 2θ , to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{\text{I}(\underline{\textbf{h}}_{\underline{\textbf{0}}})}{\text{I}_{\underline{\textbf{c}}}(113)} = \frac{\textbf{x}_{\underline{\textbf{c}}}}{\textbf{x}_{\underline{\textbf{s}}}} \cdot \frac{\text{I}_{\underline{\textbf{c}}}^{\text{rel}}(\underline{\textbf{k}})}{\text{I}^{\text{rel}}(\underline{\textbf{h}})} \cdot \frac{\text{I}(\underline{\textbf{h}})}{\text{I}(\underline{\textbf{k}})}$$

and $(\underline{h_0})$ indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection $(\underline{h_0})$ will be the one with I=100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I c. These values yield the tabulated average $\langle I/I_c \rangle$. From these data, the estimated deviation, Δ , was obtained from

$$\Delta = \frac{\sum_{i=1}^{n} |(I/I_c)_i - \langle I/I_c \rangle|}{n}$$

where n is the number of measurements of the reference intensity ratio. The estimated deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections were treated in one of two ways. If a d-spacing had only two possible indices, an M was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a + sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1."

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark et al. [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made

in the lattice constants in order to make them consistent with the revised value of $\lambda (CuK\alpha_1) =$ 1.540598A [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the convention of Crystal Data has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the International Tables for X-ray Crystallography, Vol. III, [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's (\mathring{A}^2) or the anisotropic β_{11} 's in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$
 or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters (e.g. U_{ij}) were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined

$$B = 4 \left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a*^2 b*^2 c*^2} \right]^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absoluterelative" scale is Iabs/K, as defined by Hubbard et al. [1976] in the equation

$$\frac{I_{i}^{abs}}{K} = \frac{M_{i}L_{P_{i}}|F_{i}T_{i}|^{2}}{2\mu V^{2}}$$

where:

F is the structure factor T is the thermal correction

 $Lp = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i

μ is the linear absorption coefficient

V is the volume of the unit cell.

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale (I^{rel}). Reflections with I^{rel} less than 0.7 were omitted. Relative intensities were rounded to the nearest integer value before being listed, except that for phases whose structures were postulated or were based on analogy, any intensity above 20 was rounded further, to the nearer multiple of 5.

Scale factor (integrated intensities). The scale factor, y, was defined to convert the tabulated Irel to the "absolute-relative" scale [Hubbard et al., 1976]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{K} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, k_{NBS}, was reported which is related to y:

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V^2}$$

From γ , the theoretical value of the Reference Intensity Ratio, I/I, was calculated:

$$I/I_{c} = \frac{\mu \gamma \rho_{c}}{\mu_{c} \gamma_{c} \rho}$$

where p is the density and the subscript c represents corundum $(\alpha-Al_2O_3)$.

For refined structures, the value of I/Ic was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns, I/Ic was not included.

 $\ensuremath{\text{I/I}_{c}}$ and γ are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak heights. The purpose of calculating peak height intensity was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the α_1 and the α_2 peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM)

was allowed to vary to represent the changing FWHM as a function of 20. [The values of the FWHM vs 20 are given in Table 2.]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 20 angles and produce only one composite peak in the simulated pattern. The 20 angle of the composite peak was assigned the hkl of the reflection having the greatest contribution to the peak height intensity. If any other peak contributed more than 10% of the intensity toward the composite peak height intensity, a plus sign(+) was appended to the hkl.

Peaks due solely to α_2 lines were omitted. If a composite peak was formed by the overlap of an α_1 peak of reflection <u>j</u> with the α_2 peak of reflection <u>i</u>, the reflection <u>j</u> was listed separately only if it contributed a significant intensity (>10%) at the composite peak location.

The peak search routine located peaks only at 20 angles which were a multiple of 0.02° .

Table 2

2θ CuKα ₁	FWHM	2θ CuKα ₁	FWHM
0° 20 40 60 80 100	0.12° .12 .12 .125 .130 .135 .155	140 145 150 155 160 162.5 165	0.230 .255 .285 .315 .360 .410
130	.185		

UNITS

In this publication the Angström unit (1A= 100pm) was selected for presentation of the dspacings and lattice parameters to maintain consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circu-1ar 539 volumes 1-10 and Monograph 25 sections 1-15), (b) the publications of the International Union of Crystallography: Acta Crystallographica and the Journal of Applied Crystallography, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of nearly 30,000 entries). The PDF search manuals are based on the d-spacings in A of the three strongest lines. Consistent with the choice of the A unit for length, the volume of the unit cell is expressed in A^3 (=1 x 10^{-30} m³). Other reported parameters and their units are density in g/cm^3 (1 gm/cm³ = 10⁻³ kg/m³) and the linear absorption coefficient in cm-1.

ACKNOWLEDGMENTS

We would like to thank Mary Owen of the JCPDS Associateship for her assistance, particularly for key-punching the data and helping with the proof-reading of this manuscript. Appreciation is also expressed to the Text Editing Facilities of the National Measurement Laboratory of NBS for typing the manuscript.

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CAS registry no. 103-84-4	CuKα ₁ λ	= 1.5405	98 Å; temp. 2	25±1 °C
Sample	Internal	standar	d W, a = 3.16	5524 Å
The sample is Standard Reference Material 141c of the National Bureau of Standards, obtained from J. T. Baker Co., Phillipsburg, NJ. It	d(Å)	I	hkl	2θ(°)
is used for checking microchemical procedures for the determination of carbon, hydrogen and nitrogen in organic matter.	9.81 6.82	90 30	0 2 0 1 2 0	9.01 12.97
Color Colorless	5.84 5.193 4.913	65 30 5	1 1 1 1 2 1 0 4 0	15.17 17.06 18.04
Structure Orthorhombic, Pcab (61), Z = 8. The structure was determined by Brown and Corbridge [1954] and refined by Brown [1966].	4.749 4.469 4.360 4.273 4.081	6 30 30 8 45	2 0 0 1 3 1 1 4 0 2 2 0 2 0 1	18.67 19.85 20.35 20.77 21.76
Lattice constants of this sample $a = 9.494(3) \stackrel{\circ}{A}$ $b = 19.645(4)$ $c = 7.995(2)$	3.994M 3.994M 3.917 3.826	60 55 19	0 0 2 2 1 1 0 1 2 1 4 1	22.24 22.24 22.68 23.23
a/b = 0.4833 c/b = 0.4070	3.768	40 100	2 2 1 0 2 2	23.59
Volume 0 1491. A ³	3.620 3.448 3.411M	30 55 10	1 1 2 1 2 2 2 4 0	24.57 25.82 26.10
Density (calculated) 1.204 g/cm ³	3.411M 3.305	7	0 3 2 1 5 1	26.10 26.96
Figure of merit $F_{30} = 56.3 (0.013,40)$	3.210 3.097M 3.097M	20 9	1 3 2 0 4 2 1 6 0	27.77 28.80 28.80
Reference intensity I/I corundum = 0.63(4)	2.773 2.694	5 5	2 3 2 2 6 0	32.26 33.23
Additional patterns 1. PDF card 18-1501 [Billig, B. and Greenberg, B., Polytechnic Institute of Brooklyn, 1965] 2. Morris et al. [1977]	2.658 2.597 2.549 2.543 2.535	2 8 7 8 7	3 4 0 2 4 2 1 7 1 1 1 3 0 6 2	33.69 34.51 35.18 35.27 35.38
References Brown, C. J. (1966). Acta Crystallogr. 21, 442. Brown, C. J. and Corbridge, D. E. C. (1954). Acta Crystallogr. 7, 711.	2.482 2.455 2.414 2.378 2.355	4 2 2 6 2	1 2 3 0 8 0 2 5 2 1 8 0 3 5 1	36.16 36.58 37.21 37.80 38.18
Morris, M. C., McMurdie, H. F., Evans, E. H., Paretzkin, B., de Groot, J. H., Newberry, R., Hubbard, C. R., and Carmel, S. J. (1977). Nat. Bur. Std. U.S. Monogr. 25, Sec. 14, 38.	2.308M 2.308M 2.297 2.277+ 2.277+	6 7 6	2 1 3 4 2 0 0 7 2 3 6 0 4 0 1	39.00 39.00 39.18 39.55 39.55

Acetanilide, C₈H₉NO (continued)

d(A)	I	hkl	20(°)
2.214 2.191 2.148M 2.148M 2.099	2 5 2	3 4 2 2 3 3 4 3 1 1 5 3 3 5 2	40.73 41.17 42.02 42.02 43.07
2.067 2.056 2.030M 2.030M 2.027	3 4 2	2 7 2 1 9 1 3 7 1 4 1 2 3 1 3	43.76 44.00 44.60 44.60 44.67
1.969 1.965 1.947M 1.947M 1.923M	3 2 5	4 5 1 0 10 0 3 3 3 1 1 4 4 6 0	46.05 46.17 46.62 46.62 47.23
1.923M 1.919 1.895M 1.895M 1.885M	5 4 5	1 10 0 1 2 4 2 6 3 1 7 3 3 8 1	47.23 47.32 47.98 47.98 48.24
1.885M 1.879 1.870	6 4	4 4 2 1 9 2 1 10 1	48.24 48.41 48.65

Sample
The sample was obtained from Alfa Products,
Danvers, MA.

Color Colorless

Structure Tetragonal, $I\bar{4}2d$ (122), Z=4, isostructural with KH_2PO_4 . The structure was determined by Delain [1958] and refined by Khan and Bauer [1973].

Lattice constants of this sample $a = 7.6978(6) \stackrel{\circ}{A} c = 7.7193(7)$

c/a = 1.0028

Volume 6457.41 Å³

Density (calculated) 2.308 g/cm³

Figure of merit $F_{30} = 76.2(0.012,32)$

Reference intensity
I/I = 4.3(2)

Additional pattern
1. PDF card 1-775 [Hanawalt et al., 1938]

References
Delain, C. (1958). C. R. Acad. Sci. Ser. C <u>247</u>, 1451.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. <u>10</u>, 457.
Khan, A. A. and Baur, W. H. (1973). Acta
Crystallogr. B29, 2721.

CuKα ₁ λ :	= 1.540598	8 A;	temp	٠.	25±1 °C
	standard	Ag,	a =	4.	.08651 Å
d(A)	I		hkl		2Θ(°)
5.450	80	1	0	1	16.25
3.847 3.143	65	2	0	0	23.10 28.37
2.725	100 15	2	0	2	32.84
2.719	20	2	2	0	32.91
2.438	4	1	0	3	36.83
2.433M	4	3	1	0	36.92
2.433M	•	3	Ô	1	36.92
2.058M	45	3	2	1	43.96
2.058M		3	1	2	43.96
1.929	1	0	0	4	47.07
1.924	3	4	0	0	47.20
1.8166	9	3	0	3	50.18
1.8142	9	4	1	1	50.25
1.7252	10	2	0	4	53.04
1.7218M	12	4	0	2	53.15
1.7218M		4	2	0	53.15
1.6427M	12	3	2	3	55.93
1.6427M		3	3	2	55.93
1.5738	6	2	2	4	58.61
1.5106M	11	4	1	3	61.32
1.5106M		5	0	1	61.32
1.4058M	10	5	1	2	66.45
1.4058M		5	2	1	66.45
1.3629	6	4	0	4	68.83
1.3607	4	4	4	0	68.96
1.3231	2	3	0	5	71.21
1.3213	2	4	3	3	71.32
1.2847	5	4	2	4	73.68
1.2829	3	6	0	0	73.80
1.2519	4	1	1	6	75.95
1.2489M	7	6	1	1	76.16
1.2489M		5	3	2	76.16
1.2175M	4	6	0	2	78.50
1.2175M		6	2	0	78.50
1.1900	2	4	1	5	80.68
1.1877	1	5	4	1	80.87
1.1376	2	3	1	6	85.24
1.1352M	3	6	3	1	85.46
1.1352M		6	1	3	85.46
1.1120	1L	4	4	4	87.69
1.0917	1L	1	0	7	89.76
1.0886M	3	7	1	0	90.08
1.0886M 1.0675	2	7 6	0 4	1	90.08 92.37
1.0501	2	2	1	7	94.37
1.0476M	5	7	2	1	94.66
1.0476M	_	5	5	2	94.66
1.0296	2 1T	6	2	4	96.86
1.0113	1L	7	0	3	99.23

Ammonium Titanium Fluoride, (NH₄)₂TiF₆

CAS registry no. 16962-40-7

Sample

The sample was donated by Harshaw Chemical Co., Cleveland, OH.

Color

Colorless

Structure

Hexagonal, $P\overline{3}ml$ (164), Z = 1, isostructural with K_2GeF_6 [Cox and Sharpe, 1953].

Lattice constants of this sample

 $a = 5.9456(4) \stackrel{\circ}{A}$ c = 4.8053(5)

c/a = 0.8082

Volume 03 147.11 Å³

Density

(calculated) 2.235 g/cm³

Figure of merit

 $\bar{F}_{24} = 98.9 (0.010, 25)$

Reference intensity

 $I/I_{corundum} = 1.38(7)$

Reference

Cox, B. and Sharpe, A. G.(1953). J. Chem. Soc. 1953, 1783.

CuKa ₁ /	$\lambda = 1.540598$	3 Å;	temp	. 25±1 °C	
	al standard	Ag,	a =	4.08651 Å	
d(Å)	I		hkl	20(°)
5.151	100	1	0	0 17.2	
4.808	25	0		1 18.4	
3.513	80	1	0	1 25.3	
2.972	14	1	1	0 30.0	
2.574	4	2	0	0 34.8	
2.527	6	1	1	1 35.4	
2.402	7	0	0	2 37.4	1
2.269	85	2	0	1 39.6	19
2.1767	7	1	0	2 41.4	
1.9451	2	2	1	0 46.6	
1.8686	10	1	1	2 48.6	
1.8035	14	2	1	1 50.5	
1.7569	20	2 2 3 3	0	2 52.0	
1.7165	1	3	0	0 53.3	
1.6167	4	3	0	1 56.9	
1.5293	2	1	0	3 60.4	
1.5130	9	2	1	2 61.2	
1.4863	10	2	2	0 62.4	
1.4284	3	2 2 3 2	1	0 65.2	27
1.4197	4	2	2	1 65.7	
1.4102	5	1	1	3 66.2	
1.3964	3		0	2 66.9	
1.3690	5 3 5 5	3 3 2	1	1 68.4	
1.3601	5	2	Ō	3 68.9	

Synonym 1. 4-Methoxybenzoic Acid	$CuK\alpha_1 \lambda =$					0
	Internal	standard	Si,	a =	5.43	088 A
CAS registry no. 100-09-4	d(A)	I		hkl		2Θ(°)
Sample The sample was NBS Standard Reference Material 142, a microanalytical standard for the methoxyl radical. Color Colorless Structure Monoclinic, P2 ₁ /a (14), Z = 4 [Rokade et al., 1942]. A qualitative structure was done by Richards [1956]. Lattice constants of this sample	9.18 8.40 6.69 5.48 5.221 4.598 3.924M 3.720M 3.720M 3.569M 3.569M	6 5 9 95 25 3 14 12	0 1 2 4 3 0 -2	2 1 2 1 0	0 0 0 0 0 0 0 0 1 1	9.63 10.52 13.23 16.15 16.97 19.29 22.64 22.64 23.90 23.90 24.93 24.93
$a = 16.899(4) \text{ Å}$ $b = 10.971(3)$ $c = 3.976(2)$ $\beta = 95.41(2)^{\circ}$	3.523 3.340 3.298 3.213M 3.213M	100 6 5	4 2 5	1 2 1 1 2	0 1 0	25.26 26.67 27.01 27.74 27.74
a/b = 1.5403 c/b = 0.3624 Volume 733.86 A ³	3.077 2.983 2.921 2.880	30 2 3	3 -4	2 1 1	1	29.00 29.93 30.58
Density (calculated) 1.377 g/cm ³ Figure of merit	2.869 2.802 2.754 2.745	2 3 3 2	5 6	2 0 0 4	0	31.15 31.91 32.48 32.60
F ₃₀ = 40.4(0.016,48) Additional pattern 1. PDF card 11-765 [Institute of Physics, University College, Cardiff, Wales, 1961]	2.707 2.673 2.626 2.606M 2.606M	1 5 2 3	1 2	4 1 3 4 3	1 1 0	33.06 33.50 34.12 34.38 34.38
References Richards, J. P. G. (1956). Res. Appl. Ind. 9, S44. Rokade, R. K., Khabaria, R. H., and Kapadia, M. R. (1942). J. Univ. Bombay 11, 37.	2.512 2.496 2.474 2.465M 2.465M	3 3 4 5	2 6 5 3 4	3 2 3 4 2	1 0 0 0 1	35.72 35.95 36.28 36.42 36.42
	2.416 2.398 2.392 2.365 2.348	1 1 1 1 3	-5 -6 5 3 7		1 1 1 1 0	37.19 37.47 37.57 38.01 38.31
	2.297 2.250 2.240 2.227 2.207	2 2 1 1 1	4 -1 5 6 -2	4 4 2 3 4	0 1 1 0 1	39.19 40.05 40.22 40.48 40.86

p-Anisic Acid, $C_8H_8O_3$ - (continued)

d(Å)	I		hkl		2Θ(°)
2.200M	1	7	2	0	40.99
2.200M		4	3	1	40.99
2.196	2	-6	2	1	41.06
2.176	1	1	5	0	41.47
2.169	3	- 5	3	1	41.61
2.149M	4	6	1	1	42.01
2.149M		2 5	4	1	42.01
2.125M	2	5	4	0	42.51
2.125M		2	5	0	42.51
2.102	3	8	0	0	43.00
2.065	3	8	1	0	43.81
2.043	2	3 5	5	0	44.31
2.037M	2	5	3	1	44.45
2.037M		6	2	1	44.45
2.008	1	7	3	0	45.11
1.999	1	- 7	2	1	45.32
1.969	1	-2	0	2	46.05
1.964	2	8	2	0	46.19
1.961	2 2	6	4	0	46.25
1.945M	3	4	5	0	46.67
1.945M		4	4	1	46.67

Sample

The sample was prepared by dissolving Sb metal in warm HCl and HNO₃ (both concentrated). With constant stirring, the solution was poured into water at 80 °C. Stirring was continued overnight at 70 °C. The crystals formed were filtered off and dried in air at room temperature. The water content varies somewhat but causes little change in the x-ray pattern [Abe and Ito, 1968; Stewart et al., 1972]. The material is often referred to as "Sb₂O₅·4H₂O."

Color Colorless

Structure

Cubic, Fd3m (227), Z=1. The structure was determined by Baetsle and Huys [1968]. Dehydrated phases have powder patterns similar to that of $\rm H_{14}Sb_{14}O_{21}(OH)_{42}$ in d-spacings and cell size, but are quite distinct in relative intensities [Stewart et al., 1972].

Lattice constant of this sample a = 10.3553(7) A

Volume 1110.4 Å³

Density (calculated) 4.140 g/cm³

Figure of merit F₂₀ = 54.9(0.012,31)

Reference intensity
I/I = 3.49(10)

Additional patterns

- PDF card 20-111, labeled Sb₂O₅·4H₂O [Baetsle and Huys, 1968]
- 2. PDF card 21-803, labeled Sb₂O₅·4H₂O [Abe and Ito, 1968]
- 3. Natta and Baccaredda [1936]4. Hanawalt et al. [1938]

References

Abe, M. and Ito, T. (1968). Bull. Chem. Soc. Jap. 41, 333.

Baetsle, L. H. and Huys, D. (1968). J. Inorg. Nucl. Chem. 30, 639.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Ed. 10, 457.

Natta, G. and Baccaredda, M. (1936). Gazz. Chim. Ital. 66, 308.

Stewart, D. J., Knop, O., Ayasse, C., and Woodhams, F. W. D. (1972). Can. J. Chem. 50, 690.

CuKα ₁ λ	= 1.540598	8 Å; t	em	p. 2	25±1	°C
	standard	W, a	=	3.16	5524	o A
d(Å)	I	ŀ	ıkl			2Θ(°)
5.993	100	1	1	1		14.77
3.123	70	3	1	1		28.56
2.989 2.590	90 20	2 4	2	2		29.87 34.61
2.376	10	3	3	1		37.83
2.570	10	3	J	1		37.03
2.115	3	4	2	2		42.72
1.9928	17	5	1	1		45.48
1.8302	35	4	4	0		49.78
1.7503	20	5	3	1		52.22
1.5789	10	5	3	3		58.40
1.5607	25	6	2	2		59.15
1.4950	6	4	4	4		62.03
1.4506	12	7	1	1		64.15
1.3479	10	7	3	1		69.71
1.1877	7	6	6	2		80.87
1.1576	6	8	4	0		83.43
1.1366	4	9	1	1		85.33
1.0856	2 3	9	3	1		90.40
1.0569	3	8	4	4		93.58
1.0408	4	7	7	1		95.48
1						

CAS registry no. 12165-47-8

Sample

The sample was prepared by heating antimonic acid $(H_{14}Sb_{14}O_{21}(OH)_{42})$ at 780 °C for 30 minutes

Color

Colorless

Structure

Cubic, Fd3m (227), Z = 4. Defect pyrochlore structure [Stewart et al., 1972]. This material has been reported as Sb_2O_5 [Swanson et al., 1960] and as Sb_3O_6 (OH) (stibiconite) [Dihlström and Westgren, 1937]. The composition of the mineral stibiconite is uncertain [Vitaliano and Mason, 1952].

Lattice constant of this sample a = 10.3060(2) A

Volume 0 1094.6 A³

Density

(calculated) 5.696 g/cm³

Figure of merit $F_{30} = 71.6(0.010,40)$

Additional patterns

- 1. PDF card 11-690 [Swanson et al., 1960] called $\mathrm{Sb}_2\mathrm{O}_5$
- 2. PDF card 16-938 [Dihlström and Westgren, 1937] called ${\rm Sb_3O_6(OH)}$
- 3. PDF card 21-51 [Ito et al., Tokyo Institute of Technology, 1966].
- 4. Natta and Baccaredda [1936]
- 5. Stewart et al. [1972]

References

Dihlström, K. and Westgren, A. (1937). Z. Anorg. Allg. Chem. 235, 153.

Natta, G. and Baccaredda, M. (1936). Gazz. Chim. Ital. 66, 308.

Stewart, D. J., Krop, O., Ayasse, C., and Woodhams, F. W. D. (1972). Can. J. Chem. 50, 690.

Swanson, H. E., Cook, M. I., Evans, E. H., and de Groot, J. H. (1960). Nat. Bur. Stand. U.S. Circ. 539, 10, 10.

U.S. Circ. 539, <u>10</u>, 10. Vitaliano, C. J. <u>and Mason</u>, B. (1952). Amer. Mineral. 52, 982.

CuKα ₁ λ =	= 1.54059	8 Å;	tem	p. 2	25±1 °C
	standard	W, a	= :	3.16	5524 Å
c(A)	I		hkl		20(°)
5.949	25	1	1	1	14.88
3.108	20	3	1	1	28.70
2.976	100	2	2	2	30.00
2.577	30	4	0	0	34.78
2.365	4	3	3	1	38.02
2.1022	2	4	2	2	42.99
1.9833	6	5	1	1	45.71
1.8213	25	4	4	0	50.04
1.7416	8	5	3	1	52.50
1.6293	1L	6	2	0	56.43
1.5716	2	5	3	3	58.70
1.5535	30	6	2	2	59.45
1.4876	9	4	4	4	62.37
1.4432	8	5	5	1	64.52
1.3416	6	7	3	1	70.08
1.2885	4	8	0	0	73.43
1.2592	1	7	3	3	75.43
1.1902	1	7	5	1	80.66
1.1822	8	6	6	2	81.32
1.1522	8	8	4	0	83.91
1.1313	4	9	1	1	85.83
1.0805	3	9	3	1	90.94
1.0519	6	8	4	4	94.16
1.0360	3	7	7	1	96.07
. 9965	2	9	5	1	101.25
.9918	4	10	2	2	101.92
.9611	3	9	5	3	106.54
.9291	1	11	1	1	112.00
.9109	2	8	8	0	115.49
. 9004	6	9	7	1	117.63
. 8742	6	9	7	3	123.57
.8710	8	10	6	2	124.35
. 8588	6	12	0	0	127.51
. 8500	3	11	5	1	129.98
.8277	2	11	5	3	137.06
.8148	5	12	4	0	141.96
.8072	2	9	9	1	145.20

CAS registry no. 28980-49-6

Sample

The sample was made by melting Sn and Sb together above 1100 °C in air. It was then quenched by pouring out onto a slab, and ground. This phase has a homogeneity range of 45-55 percent Sb [Hägg and Hybinette, 1935].

Color Black

Structure

Hexagonal, R**, Z = 3. This phase was studied by Hägg and Hybinette [1935]. These authors reported a rhombohedral cell with both a and c doubled. No lines were found in the authors' pattern or the NBS pattern that required the larger cell. This phase has been considered cubic [Osawa, 1929] and [Bowen and Jones, 1931].

Lattice constants of this sample

a = 4.3255(3) Å c = 5.3465(8)

c/a = 1.2360

Volume o 86.6 A³

Density

(calculated) 13.827 g/cm³

Figure of merit $F_{14} = 67.4(0.013,16)$

Reference intensity
I/I = 2.34(12)

Polymorphism

SbSn transforms to a different phase at 320 °C [Iwasê et al., 1931].

Additional patterns

1. PDF card 1-830 [Hanawalt et al., 1938]

2. Hägg and Hybinette [1935]

References

Bowen, E. G. and Jones, W. M. (1931). Phil. Mag. 12, 441.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K.

(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Hägg, G. and Hybinette, A. G. (1935). Phil.

Mag. Series 7, <u>20</u>, 913.

Iwasê, K., Aoki, N., and Osawa, A. (1931). Sc.

Rep. Tôhoku Imp. Univ. 20, 353. Osawa, A. (1929). Nature 74, 14. Internal standard W, a = 3.16524 Å

d(Å) I hkl 20(°)

3.067 100 1 0 1 29.09

 $CuK\alpha_1 \lambda = 1.540598 \text{ A}$; temp. 25±1 C

3.067	100	1	. 0	1	29.09	
2.176	30	C	1	2	41.46	
2.162	30	1	. 1	0	41.74	
1.7837	8	C	0	3	51.17	
1.7679	14	C	2	1	51.66	
1.5343	8	2	. 0	2	60.27	
1.3757	8	1	. 1	3	68.10	
1.3683	10	2	1	1	68.52	-
1.2589	3	1	. 0	4	75.45	
1.2512	7	1	. 2	2	76.00	
1.0878	1	C	2	4	90.16	
1.0814	1	2	2	0	90.85	
1.0225	2	3	0	3	97.76	
1.0200	3	1	. 3	1	98.09	

CAS registry no. 7791-28-8

Sample
The sample was made by slow evaporation of an aqueous solution at room temperature.

Color
Colorless

Optical data
Biaxial (-), N_Q = 1.720, N_β = 1.732,
N_γ = 1.748. 2V is large.

Structure

Monoclinic, C2/c (15), Z = 4. The structure was determined by Bang [1961].

Lattice constants of this sample a = 10.442(2) Å b = 7.207(1) c = 8.384(2) $\beta = 113.61(2)^{\circ}$ a/b = 1.4489

c/b = 1.1633

Volume o 578.1 Å³

Density (calculated) 3.828 g/cm³

Figures of merit $F_{30} = 82.2(0.011,32)$ $M_{20} = 43.8$

Reference intensity
I/I corundum = 4.3(2)

Reference
Bang, E. (1961). Mat. Fys. Medd. Dan. Vid.
Selsk. 33, no. 4, 1.

 $CuK\alpha_1 \lambda = 1.540598 \text{ A}$; temp. 25±1 °C Internal standard Si, a = 5.43088 A d(A) Ι hkl 2Θ(°) 5.77 25 1 1 0 15.35 5.264 20 -1 1 1 16.83 2 0 0 4.790 2 18.51 1 4.158 6 1 1 21.35 0 0 3.842M 30 23.13 3.842M -2 0 2 23.13 **-1** 1 2 10 24.55 3.623 3.606 0 2 0 24.67 16 3.265 7 0 2 1 27.29 3.134 1 -3 1 1 28.46 -2 2 1 25 30.41 2.937 2.916 45 3 1 0 30.63 100 2.890M 1 1 30.92 2.890M -3 1 30.92 0 2 2 2.629M 34.08 -2 2 2 34.08 2.629M -1 1 3 34.72 2.582 11 2 0 2 2.539M 1 35.32 -4 0 2 2.539M 35.32 2.504 16 2 2 1 35.84 3 1 1 36.71 2.446 3 -3 1 3 4 0 0 2.410 6 37.28 2.391 20 37.58 1 3 0 2.329 3 38.62 2.293 -1 3 1 39.26 16 41.11 3 -2 2 3 2.194 4 1 3 1 41.57 2.171 2.155 2 1 1 3 41.89 2.107 6 **-4** 2 1 42.89 -2 0 4 2.096 14 43.13 2.085 15 **-1** 3 2 43.36 4 4 2 0 45.48 1.993 -5 1 1 -3 3 1 -1 1 4 1.981 3 45.76 1.977 3 45.86 1.970M 4 46.03 -3 1 4 46.03 1.970M 1.911+ 9 -4 2 3 47.53 1.911+ 1 3 2 47.53 1.886 3 -5 1 3 48.22 **-1** 3 3 1.8125M 9 50.30 -2 2 4 50.30 1.8125M 4 2 1 3 3 1 4 0 2 1.7896 1 50.99 1.7641 2 51.78 1.7407M 52.53 **-**6 0 2 1.7407M 52.53 2 2 2 3 53.27 1.7182 1.7023M 9 1 1 4 53.81 1.7023M -5 1 4 53.81 2 4 0 1.6858 5 54.38 5 1 1 55.37 1.6579

CAS registry no. 13477-00-4

Sample The samp

The sample was prepared by heating $\mathrm{Ba}(\mathrm{C10}_3)_2\cdot\mathrm{H}_2\mathrm{O}$ at about 250 °C for 15 hours.

Color

Colorless

Structure

Orthorhombic. The crystal system aspect is apparently F*** and Z is assumed to be 8. The cell was determined from the Visser program [1969].

Lattice constants of this sample

a = 11.782(3) A

b = 13.264(3)c = 7.727(2)

a/b = 0.8883

c/b = 0.5826

Volume o 1207.5 A³

Density

(calculated) 3.347 g/cm^3 (assuming Z = 8)

Figure of merit

 $F_{30} = 52.2(0.014,41)$

Additional pattern

1. PDF card 1-530 [Hanawalt et al., 1938], data appears to be for Ba(ClO₄)₂

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457. Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

Internal standard Si, a = 5.43088 Å d(Å) I hk2 20(°) 5.80 80 1 1 1 15.27 4.401 8 2 2 0 20.16 3.651 60 1 3 1 24.36 3.385 95 3 1 1 26.31 3.337 100 0 2 2 26.69 3.318 45 0 4 0 26.85 3.232 25 2 0 2 27.58 2.945 20 4 0 0 30.33 2.904 9 2 2 2 2 30.76 2.889 7 2 4 0 30.93 2.745 35 3 3 1 32.59 2.473 20 1 1 3 36.30 2.454 10 1 5 1 36.59 2.314 30 2 4 2 38.88 2.221 13 5 1 1 40.59 2.210M 50 0 6 0 40.80 2.210M 4 2 2 40.80 2.188 14 1 3 3 41.22 2.126 20 3 1 3 42.49 2.114 25 3 5 1 42.73 2.070 8 2 6 0 43.70 2.007 3 5 3 1 45.14 1.936 14 3 3 3 40.24 2.114 25 3 5 1 42.73 2.070 8 2 6 0 43.70 2.007 3 5 3 1 45.14 1.936 14 3 3 3 46.89 1.919 12 0 6 2 47.34 1.884 9 6 2 0 48.28 1.8268 9 1 5 3 49.88 1.8200 10 1 7 1 50.08 1.7695 15 2 2 4 51.61 1.7509 5 6 0 2 52.20 1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 0 0 4 56.96	CuKα ₁ λ	= 1.540598	Α;	tem	p. 2	25±1 °C
d(Å) I hkl 20(°) 5.80 80 1 1 1 15.27 4.401 8 2 2 0 20.16 3.651 60 1 3 1 24.36 3.385 95 3 1 1 26.31 3.337 100 0 2 2 26.69 3.318 45 0 4 0 26.85 3.232 25 2 0 2 27.58 2.945 20 4 0 30.33 2.904 9 2 2 2 30.76 2.889 7 2 4 0 30.33 2.904 9 2 2 2 30.76 2.889 7 2 4 0 30.93 2.745 35 3 3 1 32.59 2.473 20 1 1 3 36.30 2.59 2.473 2.20 1<	Interna	l standard	Si.	a =	5.4	3088 A
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3.385 95 3 1 1 26.31 3.337 100 0 2 2 26.69 3.318 45 0 4 0 26.85 3.232 25 2 0 2 27.58 2.945 20 4 0 0 30.33 2.904 9 2 2 2 30.76 2.889 7 2 4 0 30.93 2.745 35 3 3 1 32.59 2.473 20 1 1 3 36.30 2.454 10 1 5 1 36.59 2.314 30 2 4 2 38.88 2.221 13 5 1 40.59 2.210M 50 0 6 0 40.80 2.210M 4 2 2 40.80 2.210M 4 2 2 40.80 2.188 14 1 3 3 41.22 <	3.651	60	1	3	1	
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1.936 14 3 3 3 46.89 1.919 12 0 6 2 47.34 1.884 9 6 2 0 48.28 1.8268 9 1 5 3 49.88 1.8200 10 1 7 1 50.08 1.7695 15 2 2 4 51.61 1.7509 5 6 0 2 52.20 1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 0 4 56.96						
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1.8200 10 1 7 1 50.08 1.7695 15 2 2 4 51.61 1.7509 5 6 0 2 52.20 1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 56.33 1.6154 4 4 0 4 56.96	1.8268	9	1	5	3	49.88
1.7509 5 6 0 2 52.20 1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96	1.8200	10	1			50.08
1.7509 5 6 0 2 52.20 1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96	1.7695	15	2	2	4	51.61
1.7239 4 5 1 3 53.08 1.7188 5 5 5 1 53.25 1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96	1.7509		6			
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1.6716 11 3 5 3 54.88 1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96	1 7100		_	_	1	E2 25
1.6685 13 0 4 4 54.99 1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96						
1.6319 4 7 1 1 56.33 1.6154 4 4 0 4 56.96						
1.6154 4 4 0 4 56.96						
1.6081 6 4 6 2 57.24	1.6154	4	4	0	4	56.96
	1.6081	6	4	6	2	57.24

CAS registry no. 7787-33-9

Sample

The sample was made by slow evaporation of an aqueous solution of BaI₂ at about 60 °C.

Color

Strong yellowish brown

Structure

Monoclinic, I2/a (15), Z = 4, by analogy with the powder pattern for $BaBr_2 \cdot 2H_2O$. The axial ratios confirmed those given by Groth [1906]. The equivalent C-centered cell is a = 11.090(2) A, b = 7.634(1), c = 8.656(2), β = 112.98(2)°.

Lattice constants of this sample

a = 11.089(2) Ab = 7.634(1)

b = 7.634(1)c = 8.656(2)

 $\beta = 112.96(2)^{\circ}$

a/b = 1.4526c/b = 1.1339

Volume 674.7 Å³

Density (calculated) 4.206 g/cm^3

Figure of merit F₃₀ = 68.5(0.012,38)

Reference intensity
I/I = 3.4(2)

Reference

Groth, P. (1906). <u>Chemische Krystallographie</u>
<u>I</u> (Engelmann, Leipzig, Germany), p. 242.

d(A)	I		hkl		2Θ(°)
6.12	9	1	1	0	14.47
5.518	16	0	1	1	16.05
5.110	3	2	0	0	17.34
4.386	3	-2	1		20.23
3.980M	25	0	0	2	22.32
3.980M		-2	0	2	22.32
3.819	30	0	2	0	23.27
3.765	19		1		23.61
3.443	2	-1	2	1	25.86
3.108M	60	3	1	0	28.70

	d(Å)	I		hkl		20(°)
2	3.108M		1	2	1	28.70
	3.058	30	2	2	0	29.18
	3.031M	100	1	1	2	29.45
	3.031M	200	-3	1	2	29.45
	2.756M	14	o	2	2	32.46
2	2.756M		-2	2	2	32.46
2	2.676+	10	-2	1	3	33.46
2	2.676+		2	0	2	33.46
2	2.655	13	-3	2	1	33.73
2	2.599	2	-4	1	1	34.48
_						
	2.554	15	4	0	0	35.11
	2.468	4	1 0	3	0	36.37
	2.423	12		3	1	37.07
	2.299 2.239	2	-2 3	3	1	39.16 40.25
2	233	3	5	_	1	40.23
2	2.193+	12	-1	3	2	41.13
	2.193+		2	2	2	41.13
	2.164	11	-2	0	4	41.71
2	2.122	5	4	2	0	42.56
	2.110	2	4	1	1	42.82
	2.039+	3	-1	1	4	44.39
	2.039+		-3	1	4	44.39
	2.016M	9	1	3	2	44.93
	2.016M		-3	3	2	44.93
2	2.005	6	1	2	3	45.18
,	1 0725	2	_	1	Λ	45.95
	1.9735	3 3	5 0	1 4	0	45.95 47.59
	1.9092 1.9017	3 5	- 5	2	1	47.39 47.79
	1.8828	5 7	-3 -2	2	4	48.30
	1.8722	2	-4	3	1	48.59
		_		Ū		.0,00
	1.8466M	10	4	0	2	49.31
	1.8466M		-6	0	2	49.31
	1.8068	3	- 5	2	3	50.47
	1.7972	3	1	4	1	50.76
	1.7876	6	2	4	0	51.05
				_	,	5- 4-
	1.7760M	10	1	1	4	51.41
	1.7760M		- 5	1	4	51.41
	1.7657+	5	0	2	4	51.73
	1.7657+	1	-4	2	4	51.73
	1.7364	1	- 6	1	3	52.67
	1.7011	1	6	0	0	53.85
	1.6953	4	-3	4	1	54.05
	1.6621+	14	4	2	2	55.22
	1.6621+	1-7	-6	2	2	55.22
	1.6505M	4	2	ō	4	55.64
	1.6505M		-6	0	4	55.64
	1.6389M	1	5	2	1	56.07
	1.6389M		-4	1	5	56.07
	1.6156	1L	3	2	3	56.95
	1.5921	5	5	3	0	57.87
			_	,		E0.7/
	1.5706	1	3	4	1	58.74
	1.5531+	6	6	2	0	59.47
	1.5531+	5	2 5	4 1	2	59.47 59.60
	1.5500+ 1.5500+	5	-7	1	2	59.60
	1.3300+		,	1	_	39.00

CAS registry no. 13466-21-2

Sample

The sample was prepared by heating $BaCO_3$ with $H_4P_2O_7$ at 950 °C for 1 hour, grinding and heating a few minutes at 1100 °C. Chemical analysis of material dried at 100 °C gave BaO as 68.25 percent and P_2O_5 as 31.12 percent. The theoretical composition for $Ba_2P_2O_7$ gives BaO = 68.4 percent and $P_2O_5 = 31.6$ percent.

Color Colorless

Optical data Uniaxial (+), $N_o = 1.595$, $N_e = 1.600$

Structure

Hexagonal. The crystal system aspect is apparently P63** and Z is assumed to be 3. The cell was determined from the Visser [1969] program. Ranby et al. [1955] proposed an orthorhombic cell for this phase. It did not fit our data. Mehdi et al. [1977] proposed a different orthorhombic cell which did not properly fit his data or ours.

Lattice constants of this sample

a = 9.4175(8) A c = 7.081(1)

c/a = 0.7519

Volume 543.85 Å³

Density (calculated) 4.109 g/cm³, assuming Z = 3.

Figures of merit $F_{30} = 54.8(0.012,46)$ $M_{20} = 58.7$

Reference intensity
I/I = 4.3(2)

Polymorphism

Below about 725 °C, $Ba_2P_2O_7$ forms an α phase, isostructural with α - $Ca_2P_2O_7$ [McCauley and Hummel, 1968; Ranby et al., 1955].

Additional patterns

1. PDF card 9-45 [Langguth et al., 1956]

2. Mehdi et al. [1977]

3. Ranby et al. [1955]

References

Langguth, R. P., Osterheld, R. K., and Karl-Kroupa, E. (1956). J. Phys. Chem. 60, 1335.

McCauley, R. A. and Hummel, F. A. (1968).

Trans. Brit. Ceram. Soc. 67, 624.

Mehdi, S., Hussain, M. R., and Rao, B. R. (1977). Indian J. Chem. 15A, 820.

Ranby, P. W., Mash, D. H., and Henderson, S. T. (1955). Brit. J. Appl. Phys. <u>6</u>, Sup 4, S18. Visser, J. W. (1969). J. Appl. Crystallogr. <u>2</u>,

80

 $CuK\alpha_1 \lambda = 1.540598 \text{ A}$; temp. 25±1 °C Internal standard Si, a = 5.43088 A d(A) Ι hkl 2Θ(°) 5.346 4 1 0 1 16.57 4.709 1 1 18.83 1 100 1 22.65 3.923 0 0 2 3.539 25 25.14 2 1 0 7 28.93 3.084 31.56 35 1 1 2 2.833 3 0 0 32.91 2.719 25 2.355 16 2 2 0 38.18 2 1 2 2.325 20 38.69 3 1 0 39.82 2.262 10 2.235 13 2 2 1 40.33 3 0 2 41.87 2.156M 18 3 1 1 41.87 2.156M 2,110 1 1 3 42.82 17 2 0 3 44.30 2.043 40 4 0 0 44.42 2.038 40 1.960M 7 2 2 2 46.28 4 0 46.28 1.960M 1 1 1.907 3 3 2 47.66 3 2 1.8711 4 0 48.62 7 1.8092 3 2 1 50.40 0 0 4 1.7705 5 51.58 4 1 1 1.7258 3 53.02 2 2 3 1.6671 2 55.04 1.6338 3 1 3 56.26 1.5896M 5 4 1 2 57.97 5 0 1 1.5896M 57.97 3 3 0 1 1.5694 58.79 4 2 0 1.5415 59.96 5 3 3 1 1.5327 60.34 3 4 2 1 1.5055 1L61.55 1.4829 4 3 0 4 62.59 5 1 0 1.4653 3 63.43 1.4340 5 1 1 64.98 1 1.4210 3 3 65.65 3 2 1.4130 4 2 66.07 3 1 4 67.10 1.3938 1 5 1 2 1.3540 3 69.35 1.3413M 1 5 0 3 70.10 1.3413M 0 70.10 1.3380 70.30 4 3 1 1.3170 2 71.59 4 2 3 1.2903 1 73.31 1.2856 73.62

CAS registry no. 13466-25-6	d(A)
Sample The sample was made by adding a concentrated solution of Na ₂ S ₂ O ₃ to a similar hot solution of BaCl ₂ . The solution was then cooled. This produced small plates. When the pure material was dissolved in water and the	3.468 3.386 3.342 3.244 3.235M
liquid allowed to evaporate at room temperature, small needles were formed. The intensities were determined on a mixture of the crystal types.	3.235M 3.190 3.162 3.077 2.973
Color Colorless	2 022
Structure Orthorhombic, Pnca (60), Z = 8. The structure of BaS ₂ O ₃ ·H ₂ O was studied by Nardelli and Fava [1962].	2.922 2.748 2.715M 2.715M 2.661
	2.577
Lattice constants of this sample a = 7.386(1) A b = 20.050(3) c = 7.191(2)	2.554 2.508 2.479 2.449
a/b = 0.3684 c/b = 0.3587	2.382 2.343 2.314
Volume o 1064.9 A ³	2.292 2.263
Density (calculated) 3.337 g/cm ³	2.254M 2.254M 2.223
Figure of merit F ₃₀ = 51.4 (0.015,40)	2.199 2.166
Additional pattern	2.146
1. PDF card 1-42 [Hanawalt et al., 1938]	2.128 2.112
References Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed.	2.076 2.057M
10, 457. Nardelli, M. and Fava, G. (1962). Acta Crystallogr. 15, 477.	2.057M 2.040 2.006 1.916 1.869
CuKα ₁ λ = 1.540598 Å; temp. 25±1 °C	1.847
Internal standard Ag, a = 4.08651 Å	1.839M 1.839M 1.8071
d(Å) I hkl 20(°)	1.7619

1. PDF card 1- References Hanawalt, J. I L. K. (1938) 10, 457. Nardelli, M. a Crystallogr)., Rinn,). Ind. I	H. W Eng. (., Che	and m. A	Frevel, Anal. Ed.
	= 1.54059	Ť		_	0
	standar	Ag,	a	- 4.	A 10000
d(A)	I	1	hkl		2Θ(°)
10.04	9	0	2	0	8.80
5.018	60			0	17.66
4.900	7		3		18.09
4.588	35	1	2	1	19.33
4.085	5	1	3	1	21.74
3.694	50	2 2	0	0	24.07
3.630	50	2	1	-	24.50
3.594M	100	0	0	2	24.75
3.594M		1	4	1	24.75
3.501	10	0	5	1	25.42
					ļ

d(Å)	I	hkl	2Θ(°)
3.468 3.386 3.342 3.244 3.235M	20 25 75 11 16	2 2 0 0 2 2 0 6 0 2 1 1 1 0 2	25.67 26.30 26.65 27.47 27.55
3.235M 3.190 3.162 3.077 2.973	25 5 8 16	2 3 0 1 1 2 1 5 1 1 2 2 2 4 0	27.55 27.95 28.20 29.00 30.03
2.922 2.748 2.715M 2.715M 2.661	25 10 12	0 4 2 2 4 1 1 4 2 2 5 0 0 7 1	30.57 32.56 32.97 32.97 33.65
2.577 2.554 2.508 2.479 2.449	35 30 30 55 55	2 0 2 2 1 2 0 8 0 2 6 0 0 6 2	34.78 35.11 35.78 36.21 36.66
2.382 2.343 2.314 2.292 2.263	6 6 16 20 45	0 1 3 2 6 1 3 1 1 2 4 2 2 7 0	37.73 38.39 38.88 39.28 39.80
2.254M 2.254M 2.223 2.199 2.166	55 30 18 14	1 8 1 0 3 3 1 2 3 3 3 1 2 5 2	39.96 39.96 40.55 41.01 41.66
2.146 2.128 2.112 2.076 2.057M	10 2 7 15 10	1 7 2 0 9 1 3 4 1 1 4 3 0 5 3	42.08 42.45 42.78 43.56 43.99
2.057M 2.040 2.006 1.916 1.869	35 9 11 12	0 8 2 2 6 2 0 10 0 2 7 2 1 10 1	43.99 44.38 45.17 47.40 48.69
1.847 1.839M 1.839M 1.8071 1.7619	5 8 7 12	4 0 0 4 1 0 0 7 3 3 7 1 2 10 0	49.31 49.54 49.54 50.46 51.85
1.7512 1.7401 1.7355 1.6863 1.6707	11 8 7 6 12	0 10 2 1 1 4 3 6 2 1 8 3 0 12 0	52.19 52.55 52.70 54.36 54.91
1.6341M 1.6341M 1.6159M 1.6159M 1.6102	18 10 12	2 11 0 4 5 1 2 0 4 4 6 0 3 9 1	56.25 56.25 56.94 56.94 57.16

Barium Thiosulfate Hydrate, $BaS_2O_3 \cdot H_2O$ (continued)

d(Å)	I	hkl	2Θ(°)
1.6010 1.5824M 1.5824M 1.5514 1.5220	10 18 7 18	1 5 4 0 6 4 2 10 2 4 7 0 2 12 0	57.52 58.26 58.26 59.54 60.81
1.5146 1.4876 1.4229M 1.4229M	17 8 14	0 12 2 2 11 2 1 11 3 2 13 0	61.14 62.37 65.55 65.55

	CuKα ₁ λ	= 1.540598	8 A;	tem	p. 25±	1 °C
Synonym 1. 2-Bromobenzoic Acid		l standard	Si,	a =	5.430	88 Å
CAS registry no. 88-65-3	d(A)	I		hkl		2Θ(°)
Sample	11.41 7.41	13 5	2			7.74 11.94
The sample was NBS Standard Reference Material 2142.	6.56 5.905 5.716	55 80 25	-2 2 4	0 0 0	2 2 0	13.49 14.99 15.49
Color Colorless	4.805 4.290	4 40	- 4		2	18.45 20.69
Structure Monoclinic, A2/a (15), $Z = 8$. The structure was determined by Ferguson and Sim [1962].	3.940 3.862 3.811	30 60 40		1 1	1	22.55 23.01 23.32
Lattice constants of this sample a = 23.016(4) A b = 4.085(1)	3.756 3.691M 3.691M 3.641	25 90 45				23.67 24.09 24.09 24.43
c = 14.871(3) β = 96.62(2)°	3.558	65	- 6	0	2	25.01
a/b = 5.6343 c/b = 3.6404	3.454 3.401 3.288 3.237	19 18 100 14	3 2 -4 6	0 1	1 4 1 2	25.77 26.18 27.10 27.53
Volume 0 1389.0 A ³	3.198	30	4	1	1	27.88
Density (calculated) 1.923 g/cm ³	3.144M 3.144M 3.088M	5 17		1 1 1		28.36 28.36 28.89
Figure of merit $F_{30} = 68.6(0.012,37)$	3.088M 3.033	6	-5	1	3	28.89 29.43
Reference intensity I/I = 0.80(2)	2.982 2.974 2.950	20 17 12	2 4	1 1 0	3 4	29.94 30.02 30.27
Additional pattern 1. PDF card 13-794 [Ferguson and Sim, 1959]	2.856	40 19	-6	0	0	31.29 32.16
Reference Ferguson, G. and Sim, G. A. (1962). Acta Crystallogr. <u>15</u> , 346.	2.696 2.673 2.569 2.511 2.465	11 25 14 30 19		0	3	33.20 33.50 34.90 35.73 36.42
	2.388 2.352M 2.352M 2.347M 2.347M	25 9 7	2 -7	1 0 1 1	6 3 1	37.63 38.23 38.23 38.32 38.32
	2.300 2.280 2.259 2.226 2.186M	6 19 4 4 8	2 8 -10 3 7		1	39.13 39.49 39.87 40.49 41.26
	2.186M 2.139 2.115 2.106 2.052M	9 6 6 8	-6 4 10 9 -9	1 0	6 5 2 1 3	41.26 42.22 42.71 42.91 44.10

o-Bromobenzoic Acid, $C_7H_5BrO_2$ - (continued)

0					
d(Å)	I	1	hkl		20(°)
2.052M		-10	0	4	44.10
1.981	5	-8	0	6	45.76
1.967M	18	- 1.	2	2	46.12
1.967M		6	0	6	46.12
1.950M	11	-2	2	2	46.54
1.950M		10	1	1	46.54
1.9264	10	-8	1	5	47.14
1.9237	9	4	2	0	47.21
1.9047	4	12	0	0	47.71
1.8835	11	-1	1	7	48.28
1.8751	9	0	1	7	48.51
1.8568	5	-2	0	8	49.02
1.8497M	5	7	1	5	49.22
1.8497M		10	0	4	49.22
1.8385	5	-4	1	.7	49.54
1.8282M	7	- 5	2	2	49.84
1.8282M		-9	1	5	49.84
1.8200M	8	-4	0	8	50.08
1.8200M		2	1	7	50.08
1.8005M	6	6	2	0	50.66
1.8005M		-5	1	7	50.66
1.7955M	10	12	0	2	50.81
1.7955M		-11	1	3	50.81
1.7880+	12	10	1	3 2	51.04
1.7880+		5	2	2	51.04
1.7670	8	8	0	6	51.69
1.7559M	6	8	1	5	52.04
1.7559M		-6	1	7	52.04

Sample

The sample was prepared by heating CdO and $\mathrm{B}_2\mathrm{O}_3$ in a 1:2 molar mixture at 900 °C for 5 hours.

Color

Colorless

Structure

Orthorhombic, Pbca (61), Z = 8, [Hand and Krogh-Moe, 1962]. The structure of CdB₄O₇ has been determined by Ihara and Krogh-Moe [1966].

Lattice constants of this sample

a = 8.704(1) A

b = 14.176(2)

c = 8.229(1)

a/b = 0.6140

c/b = 0.5805

Volume

1015.4 Å³

Density

(calculated) 3.501 g/cm³

Figure of merit

 $F_{30} = 50.8(0.013,46)$

Reference intensity

 $I/I_{corundum} = 0.82(6)$

Additional pattern

1. PDF card 14-162 [Hand and Krogh-Moe, 1962]

References

Hand, D. and Krogh-Moe, J. (1962). J. Amer.

Ceram. Soc. 45, 197.

Ihara, M. and Krogh-Moe, J. (1966). Acta

Crystallogr. 20, 132.

CuKα ₁ λ :	= 1.54059	8 Å;	tem	p. 2	5±1 °C
Internal	standard	W, a	=	3.16	524 Å
d(A)	I	hk	l L		2Θ(°)
7.10	12	0	2	0	12.45
5.504	70	1	1	1	16.09
5.371	100	0	2	1	16.49
4.574	11	1	2	1	19.39
4.164	50	2	1	0	21.32
4.113	30	0	0	2	21.59
3.717M	80	1	0	2	23.92
3.717M		2	1	1	23.92
3.599	60	1	1	2	24.72
3.555	45	0	2	2	25.03

d(Å)	I	hkl	2θ(°)
3.544 3.202 2.984 2.924M 2.924M	45 95 30 70	0 4 0 2 3 0 2 3 1 2 1 2 1 3 2	25.11 27.84 29.92 30.55 30.55
2.749 2.687M 2.687M 2.559 2.527	20 19 85 2	2 4 0 3 1 1 0 4 2 0 2 3 2 3 2	32.54 33.32 33.32 35.04 35.49
2.456 2.372 2.338 2.290M 2.290M	13 25 5 40	1 2 3 3 0 2 3 1 2 2 1 3 1 3 3	36.56 37.90 38.47 39.32 39.32
2.282 2.272 2.255 2.197 2.176	60 20 8 10 25	2 5 1 0 6 1 1 5 2 1 6 1 4 0 0	39.45 39.63 39.95 41.04 41.46
2.120 2.082M 2.082M 2.059M 2.059M	4 6 16	3 3 2 2 3 3 4 1 1 2 5 2 0 0 4	42.61 43.42 43.42 43.94 43.94
2.016 1.994 1.970M 1.970M 1.918M	30 5 55 14	4 2 1 1 6 2 3 4 2 3 5 1 3 2 3	44.93 45.46 46.03 46.03 47.35
1.918M 1.8540M 1.8540M 1.8438M 1.8438M	20 20	1 7 1 4 4 0 2 6 2 2 1 4 1 3 4	47.35 49.10 49.10 49.39 49.39
1.8361M 1.8361M 1.7958 1.7916 1.7785M	30 30 20 30	3 3 3 2 7 0 2 5 3 2 7 1 0 4 4	49.61 49.61 50.80 50.93 51.33
1.7785M 1.7718 1.7531 1.7435 1.7306	20 4 2 25	1 7 2 0 8 0 1 6 3 1 4 4 2 3 4	51.33 51.54 52.13 52.44 52.86
1.6988 1.6912M 1.6912M 1.6744 1.6577	4 8 8 18	1 8 1 5 1 1 4 4 2 3 6 2 4 2 3	53.93 54.19 54.19 54.78 55.38
1.6274M 1.6274M 1.6066 1.6023 1.6002M	3 7 9 11	3 7 1 0 8 2 1 1 5 5 3 1 4 6 0	56.50 56.50 57.30 57.47 57.55

Cadmium Borate, CdB_4O_7 - (continued)

d(A)	I	hkl	2Θ(°)
1.6002M	7	1 8 2	57.55
1.5926M	7	5 1 2 4 5 2	57.85
1.5926M	5	4 5 2 1 2 5	57.85
1.5765	10	4 6 1	58.50 58.74
1.3700	1.0	4 0 1	
1.5552	5	2 5 4	59.38
1.5512	4	0 6 4	59.55
1.5399	4	3 7 2	60.03
1.5302M	6	2 1 5	60.45
1.5302M		1 3 5	60.45
1.5234M	11	3 6 3	60.75
1.5234M		1 9 1	60.75
1.5188	13	5 3 2	60.95
1.4943	5 7	4 0 4	62.06
1.4876M	7	0 8 3	62.37
1.4876M		3 8 1	62.37
1.4624M	1.1	4 2 4	63.57
1.4624M		5 1 3	63.57
1.4601M	15	5 4 2	63.68
1.4601M		5 5 1	63.68
1.4428	3	6 1 0	64.54
1.4208M	6	6 2 0	65.66
1.4208M		3 7 3	65.66
1.4176	7	0 10 0	65.83
1.4032M	10	5 3 3	66.59
1.4032M		3 2 5	66.59
1.3958	4	5 5 2	66.99
1.3869	5	6 3 0	67.48
1.3818M	7	4 6 3	67.76
1.3818M		5 6 1	67.76
1.3777	10	4 4 4	67.99
1.3740	9	4 8 0	68.20
1.3699M	14	3 3 5	68.43
1.3699M		2 7 4	68.43

Sample
The sample was prepared by heating a 1:1
molar mixture of $CdCO_3$ and $(NH_4)_2HPO_4$ at
700 °C for several days, followed by
heating at 800 °C for 2 hours.

Color Colorless

Structure

Triclinic, $P\bar{1}$ (2), Z = 2. The structure of $Cd_2P_2O_7$ was determined by Calvo and Au [1969].

Lattice constants of this sample

a = 6.602(2) Ab = 6.778(2)

c = 6.631(2)

 $\alpha = 95.79(2)^{\circ}$

 $\beta = 97.68(2)$

y = 65.00(2)

a/b = 0.9740

c/b = 0.9783

Volume o 266.2 Å³

Density

(calculated) 4.975 g/cm³

Figure of merit $F_{30} = 51.3(0.012,47)$

Reference intensity $I/I_{corundum} = 1.58(3)$

Additional patterns

1. PDF card 17-635 [Brown and Hummel, 1964]

2. Ropp et al. [1961]

References

Brown, J. J. and Hummel, F. A. (1964). J.

Electrochem. Soc. $\underline{111}$, 1052. Calvo, C. and Au, P. \overline{K} . L. (1969). Can. J.

Chem. <u>47</u>, 3409. Ropp, R. C., Mooney, R. W., and Hoffman, C. W. W. (1961). Anal. Chem. <u>33</u>, 1687.

CuKα ₁ λ	= 1.54059	8 Å;	tem	p. :	25±1 °C
Internal standard Ag, a = 4.08651 Å					
d(A)	I		hkl		2Θ(°)
6.15	12	0	1	0	14.40
5.965	8	1	0	0	14.84
4.645	11	-1	0	1	19.09
4.586	18	-1	-1	1	19.34
4.377	15	0	1	1	20.27

	2-2-7			
	d(A)	I	hkl	2Θ(°)
	4.207	40	1 0 1	21.10
	3.987	14	1 1 1	22.28
	3.353	30	1 2 0	26.56
	3.279	25	0 0 2	27.17
	3.262	35	2 1 0	27.32
	3.202	33	2 1 0	21.32
	3.194	35	-1 1 1	27.91
	3.126	35	-1 -2 1	28.53
	3.094	100	-2 -1 1	28.83
	3.068	85	0 2 0	29.08
	2.974	45	2 0 0	30.02
	2.956	80	0 -1 2	30.21
	2.835M	90	0 1 2	31.53
	2.835M		0 -2 1	31.53
	2.794	7	2 2 0	32.01
	2.729	8	0 2 1	32.79
	2.708	5	-2 -2 1	33.05
	2.671	10	1 1 2	33.53
	2.613	20	2 0 1	34.29
	2.489	14	-2 -1 2	36.05
	2.449	30	2 2 1	36.66
	2.325M	30	-2 1 0	38.69
	2.325M		-2 0 2	38.69
	2.298	14	0 -2 2	39.17
	2.240	4	1 3 0	40.23
	2.218	20	1 -2 1	40.65
	2.187M	6	0 2 2	41.25
	2.187M		0 0 3	41.25
	2.170M	30	3 1 0	41.58
	2.170M		2 1 2	41.58
	2.142	16	-1 -1 3	42.16
	2.124	30	-1 0 3	42.52
	2.114	17	3 2 0	42.73
	2.101M	12	2 0 2	43.01
	2.101M		-3 -2 1	43.01
	1.993	6	2 2 2	45.47
	1 07/	,	2 2 1	/F 00
	1.974	4	2 3 1	45.93
	1.9526	14	-2 1 2	46.47
	1.9470	16	1 1 3	46.61
	1.9256M	18	0 3 1	47.16
	1.9256M		-3 -1 2	47.16
	1.8961	4	-1 1 3	47.94
	1.8526	18	-2 -2 3	47.94
	1.8526 1.7756M	18		51.42
	1.7756M	14	0 - 3 2 1 3 2	51.42
	1.7756H 1.7264M	14	-1 3 0	53.00
	1./20411	14	-1 3 0	33.00
	1.7264M		-3 -3 2	53.00
	1.7117M	14	2 1 3	53.49
	1.7117M	14	3 1 2	53.49
	1.6982	8	0 3 2	53.95
				55.55
				

Sample		
The sample	was	prepared by heating a 3:2 molar
mixture of	CdO	and (NH ₄) ₂ HPO ₄ at 800 °C over-
night.		

Color Colorless

Structure

Monoclinic, $P2_1/c$ (14), Z=4. The cell was found by use of the Visser program [1969] and by comparison with β - $Zn_3(P0_4)_2$ and $Mn_3(P0_4)_2$. The space group was assigned by consideration of the absences in the powder pattern.

Lattice constants of this sample

a = 8.662(2) A b = 10.333(3) c = 8.307(2)

 $\beta = 114.48(2)^{\circ}$

a/b = 0.8383c/b = 0.8039

Volume 676.7 A³

Density (calculated) 5.174 g/cm^3 (assuming Z = 4)

Figures of merit $F_{30} = 72.4(0.011,39)$ $M_{20} = 35.5$

Reference intensity
I/I = 1.16(6)

Additional pattern
1. PDF card 14-443 [Ropp et al., 1962]

References

Ropp, R. C., Mooney, R. W., and Hoffman, C. W. W. (1961). Anal. Chem. 33, 1687.

Visser, J. W. (1969). J. Appl. Crystallogr. 2,

CuKα ₁ λ	= 1.540598	ßÅ;	tem	р.	25±1 °C
Interna	l standard	Ag,	a =	4.	.08651 Å
d(A)	I		hkl		2Θ(°)
7.87	2	1	0	0	11.23
6.27	4	1	1	0	14.12
6.10	6	0	1	1	14.50
4.318	50	1	2	0	20.55
4.263	25	0	2	1	20.82
4.195	14	1	1	1	21.16
3.969	25	-2	1	1	22.38
3.942	9	2	0	0	22.54
3.844	30	-1	1	2	23.12
3.778	19	0	0	2	23.53

3 (4 / 2				
d(Å)	I	hk	ı	2Θ(°)
3.562 3.429 3.367 3.305 3.230	30 80 90 100 18	-2 0 1 2 -2 1 -2 2 -1 2	2 1 2 1 2	24.98 25.96 26.45 26.96 27.59
3.154 3.101 3.051 2.962 2.933	60 25 30 85 16	1 3 -1 3 0 2 1 0 -2 2	0 1 2 2 2	28.27 28.77 29.25 30.15 30.45
2.898 2.848 2.775 2.753 2.663M	35 18 3 3 45	2 1 1 1 -3 1 1 3 -1 1	1 2 1 1 3	30.83 31.38 32.23 32.50 33.63
2.663M 2.650 2.627 2.594 2.546M	50 30 45 8	-3 1 -1 3 3 0 2 3 0 3	2 2 0 0 2	33.63 33.80 34.10 34.55 35.22
2.546M 2.516 2.477 2.449 2.431M	18 4 25 25	3 1 -3 2 -2 3 0 1 -1 2	0 1 2 3 3	35.22 35.65 36.24 36.66 36.94
2.431M 2.385 2.317 2.270 2.265	2 4 4 3	-3 2 -2 2 -3 1 2 3 0 2	2 3 3 1 3	36.94 37.69 38.84 39.67 39.76
2.251 2.213 2.152M 2.152M 2.106	1L 3 12	1 4 -2 4 -1 3 -4 0 -4 1	1 1 3 2 2	40.02 40.74 41.95 41.95 42.91
2.099 2.092M 2.092M 2.073 2.034M	10 12 3 16	2 2 -2 4 -4 1 -2 0 0 3	2 2 1 4 3	43.05 43.20 43.20 43.63 44.51
2.034M 1.994 1.987 1.971M 1.971M	15 16 25	3 2 0 5 -4 2 -4 1 4 0	1 1 2 3 0	44.51 45.45 45.63 46.00 46.00
1.936M 1.936M 1.923M 1.923M 1.910	17 13 25	4 1 -3 1 -3 4 -2 2 2 3	0 4 1 4 2	46.90 46.90 47.23 47.23 47.57
1.885M 1.885M 1.8632M 1.8632M 1.8424M	15 8 12	1 5 -1 4 -2 5 -2 4 3 4	1 3 1 3 0	48.24 48.24 48.84 48.84 49.43
1.8424M		4 2	0	49.43

Calcium Aluminum Iron Oxide (Brownmillerite), Ca4Al2Fe2O10

CAS registry no. 12068-35-8

Sample

The sample was prepared by the Portland Cement Association. This phase is a component of portland cement and is known as C_4AF .

Color

Deep brown

Structure

Orthorhombic, Pcmn (62), Z = 2. The structure was determined by Bertaut et al. [1959]. $Ca_4Al_2Fe_2O_{10}$ is isostructural and forms a series of solid solutions with $Ca_2Fe_2O_5$ [Bertaut et al., 1959].

Lattice constants of this sample

a = 5.5672(9) Ab = 14.521(2)

c = 5.349(1)

a/b = 0.3834c/b = 0.3684

Volume 6432.4 A3

Density (calculated) 3.732 g/cm³

Figure of merit F₃₀ = 30.9(0.011,85)

Reference intensity
I/I corundum = 1.32(10)

Additional patterns

1. PDF card 11-124 [Midgley, 1957]

2. Bertaut et al. [1959]

3. Hansen et al. [1928]

References

Bertaut, E. F., Blum, P., and Sagnieres, A. (1959). Acta Crystallogr. 12, 149.

Hansen, W. C. and Brownmiller, S. T. (1928).

Amer. J. Sci. <u>15</u>, 224.

Midgley, H. G. (1957). Mag. Concr. Res. March 1957.

CuKα ₁ λ	L = 1.54059	98 A	; t	emp	. 25±1 °C
	ıl standar	d W,	a :	= 3	.16524 Å
d(Å)	I		hkl		2Θ(°)
7.25	45	0	2	0	12.20
5.193	4	1	1	0	17.06
3.859	4	1	0	1	23.03
3.654	16	1	3	0	24.34
3.629	6	0	4	0	24.51
3.406	4	1	2	1	26.14
2.784	25	2	0	0	32.12
2.673	35	0	0	2	33.50
2.644	100	1	4	1	33.88
2.576	17	1	5	0	34.80
2.472	2	2	0	1	36.32
2.434	4	2	1	1	36.90
2.210	8	2	4	0	40.79
2.155	9	0	4	2	41.89
2.051	35	1	6	1	44.13
1.9283	35	2	0	2	47.09
1.8813	3	2	5	1	48.34
1.8632	9	2	2	2	48.84
1.8149	45	0	8	0	50.23
1.7952	3	0	6	2	50.82
1.7327	7	3	3	0	52.79
1.5784	14	3	4	1	58.42
1.5638	4	3	5	0	59.02
1.5380	14	1	4	3	60.11
1.5202	7	2	8	0	60.89
1.5013+	8	2	0	3	61.74
1.5013+		3	5	1	61.74
1.4524	4		10	0	64.06
1.4197	5	3	6	1	65.72
1.3901	6	1	6	3	67.30
1.3669	3	4	2	0	68.60
1.3588	5	1	10	1	69.07
1.3373	4	0	0	4	70.34
1.3215	12	2	8	2	71.31

 $CuK\alpha$, $\lambda = 1.5/0508$ A. town 25+1.90

CAS registry no. 12007-99-7

Sample
The sample was obtained from Alfa Products
(Ventron), Danvers, MA.

Color Dark olive brown

Structure
Cubic, Pm3m (221), Z = 1. The structure was
determined by von Stackelberg and Newmann [1932].

Lattice constant of this sample a = 4.1535(1) Å

Volume 71.653 Å³

Density (calculated) 2.432 g/cm³

Figure of merit F₂₁ = 74.2(0.012,24)

Reference intensity
I/I = 1.92(10)

Additional pattern
1. PDF card 3-654 [von Stack

1. PDF card 3-654 [von Stackelberg and Neumann, 1932].

Reference

von Stackelberg, M. and Neumann, F. (1932). Z. Phys. Chem. 19, 314.

CuKα ₁ λ	= 1.540598	Ä;	ter	np.	25 ± 1	°C
i	l standard	W, a	=	3.1	6524	o A
d(Å)	I		hk	2		2Θ(°)
4.151	6	1	0	0		21.39
2.938	100	1	1	0		30.40
2.398	45	1	1	1		37.48
2.077	25	2	0	0		43.53
1.8572	30	2	1	0		49.01
1.6953	5	2	1	1		54.05
1.4686	5 3	2	2	0		63.27
1.3847	19	3	0	0		67.60
1.3137	13	2 2 3 3	1	0		71.80
1.2523	4	3	1	1		75.92
1.1522	1	3	2	0		83.91
1.1100	4	3	2	1		87.89
1.0384		4	0	ō		95.77
1.0073	2 3	4	1	0		99.76
.9791	4	4	1	1		103.76
.9528	1L	3	3	1		107.89
.9287		4	2	Ô		112.09
.9064	2 4	4	2	1		116.38
.8856	2	3	3	2		120.87
.8146	4	5	1	0		142.05
.0140	4	J	1	U		142.03
.7993	3	5	1	1		149.04

Synonym 1. 3-Chlorobenzoic Acid
CAS registry no. 535-80-8
Sample The sample was NBS Standard Reference Material 2144.
Color Colorless
Structure Monoclinic, $P2_1/a$ (14), $Z = 4$. The structure was determined by Gougoutas and Lessinger [1975]
Lattice constants of this sample a = 11.110(2) Å b = 16.015(3) c = 3.8455(8) β = 95.00(2)°
a/b = 0.6937 c/b = 0.2401
Volume 681.6 A ³
Density (calculated) 1.526 g/cm ³
Figure of merit F ₃₀ = 53.8(0.011,52)
Reference intensity I/I = 0.63(7)
Additional patterns 1. PDF card 24-1594 [Li, Polytechnic Institute of Brooklyn, Brooklyn, NY.] 2. PDF card 20-1577 [Dept. of Physics, Univ. Coll., Cardiff, Wales.]
Reference Gougoutas, J. Z. and Lessinger, L. (1975). J. Solid State Chem. 12, 51.

d(Å)	I		hkl		2Θ(°)
9.07	6	1	1	0	9.74
6.48	85	1	2	0	13.65
5.538	7	2			15.99
4.808	55	1	3	0	18.44
4.549	16	2	2	0	19.50

d(A)	I	hkl	2Θ(°)
4.005 3.842 3.622 3.591 3.453	18 45 45 16 35	0 4 0 2 3 0 -1 1 1 3 1 0 0 2 1	22.18 23.13 24.56 24.77 25.78
3.376 3.351 3.287 3.243 3.220	100 14 75 95 90	-1 2 1 3 2 0 -2 0 1 2 4 0 -2 1 1	26.38 26.58 27.11 27.48 27.68
3.114 3.077 3.041 2.799 2.771M	9 12 5 10	0 3 1 1 5 0 -2 2 1 -2 3 1 2 5 0	28.64 29.00 29.35 31.95 32.28
2.771M 2.727M 2.727M 2.670 2.629	8 12 4	0 4 1 4 1 0 -1 4 1 0 6 0 -3 2 1	32.28 32.82 32.82 33.54 34.07
2.615 2.516 2.456M 2.456M 2.416M	4 8 20 25	4 2 0 3 1 1 4 3 0 0 5 1 2 4 1	34.26 35.65 36.56 36.56 37.18
2.416M 2.342 2.301 2.276 2.240	2 4 5 1	3 5 0 -4 0 1 3 3 1 4 4 0 1 7 0	37.18 38.41 39.11 39.57 40.23
2.201 2.192 2.168 2.162 2.156	2 3 8 9 8	2 5 1 5 1 0 -1 6 1 3 6 0 4 0 1	40.98 41.14 41.63 41.74 41.87
2.134 2.113 2.044 2.002M 2.002M	7 3 4 13	5 2 0 2 7 0 5 3 0 2 6 1 0 8 0	42.31 42.75 44.27 45.25 45.25
1.971 1.9376 1.9214 1.8983 1.8788	2 2 2 3 6	1 8 0 5 4 0 4 6 0 4 4 1 -2 7 1	46.02 46.85 47.27 47.88 48.41
1.8326 1.7635+ 1.7635+ 1.7597m 1.7597M	2 9 9	6 1 0 2 0 2 4 7 0 3 8 0 -4 6 1	49.71 51.80 51.80 51.92 51.92
1.7432 1.6930M 1.6930M 1.6747+ 1.6747+	7 7 4	6 3 0 -5 5 1 2 9 0 -3 3 2 2 3 2	52.45 54.13 54.13 54.77 54.77

Synonym 1. Dichlorotetraaquochromium(III) chloride dihydrate, [Cr(H ₂ O) ₄ Cl ₂]Cl·2H ₂ O
CAS registry no. 10060-12-5
Sample The sample was obtained from City Chemical Corp., New York, NY.
Color Very dark yellowish green
Structure Monoclinic, C2/c (15), Z = 4. The structure was determined by Dance and Freeman [1965]. Morosin [1966] had also independently determined the same structure. The synonym name and formula are those obtained as the results of crystal structure analysis.
Lattice constants of this sample
a = 12.048(2) \mathring{A} b = 6.8352(8) c = 11.643(1) $\mathring{\beta}$ = 94.14(1)°
a/b = 1.7626 c/b = 1.7032
Volume 956.27 Å ³
Density (calculated) 1.851 g/cm ³
Figure of merit F ₃₀ = 65.2(0.012,39)
Polymorphism A hexagonal modification has been reported by Andress and Carpenter [1934].
Additional pattern 1. PDF card 12-446 [Shrier, Rutgers University]
References Andress, K. R. and Carpenter, C. (1934) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 87A, 446. Dance, I. G. and Freeman, H. C. (1965). J. Inorg. Chem. 4, 1555. Morosin, B. (1966). Acta Crystallogr. 21, 280.

CuKa ₁	$\lambda = 1.540598$	8 Å;	temj	p. 25	5±1 °C
	rnal standard	Si,	a =	5.43	8088 Å
d(A)	I		hkl		2Θ(°)
6.00 5.805 5.362 5.211 4.333	45 30 100 65 30	2 0 -1 1 -2	0 0 1 1 0	0 2 1 1 2	14.74 15.25 16.52 17.00 20.48
4.079 4.032 3.456 3.371 3.297	18 16 30 55 25	1 2 3 -3 -1	1 0 1 1	2 2 0 1 3	21.77 22.03 25.76 26.42 27.02
3.278 3.054 3.006 2.946 2.902M	30 40 6 40 17	0 -3 4 0 -2	2 1 0 2 2	1 2 0 2 1	27.18 29.22 29.70 30.32 30.79
2.902M 2.893 2.853 2.749 2.690	14 13 19 30	0 3 2 -4 -2	0 1 2 0 0	4 2 1 2 4	30.79 30.88 31.33 32.54 33.28
2.682 2.644 2.605 2.592 2.571	25 6 25 30 40	-2 -1 2 4	2 1 2 0 1	2 4 2 2 4	33.38 33.87 34.40 34.58 34.87
2.543 2.500 2.398 2.294 2.268	9 8 8 2 3	2 3 -2 -3 5	0 1 2 1 1	4 3 3 4 0	35.27 35.89 37.48 39.24 39.71
2.256M 2.256M 2.238M 2.238M 2.212	6 6 5	4 -5 -4 1 0	2 1 2 3 2	0 1 1 0 4	39.93 39.93 40.27 40.27 40.76
2.204 2.194M 2.194M 2.189 2.167	5 9 8 8	-1 4 1 -1 -4	3 2 3 1 0	1 1 1 5 4	40.91 41.11 41.11 41.20 41.64
2.138 2.115 2.080 2.066M 2.066M	15 3 2 7	1 -2 1 4 5	1 2 3 2 1	5 4 2 2 2	42.24 42.71 43.47 43.78 43.78
2.040 2.017M 2.017M 1.997 1.980	20 10 4 3	2 -5 4 -4 3	2 1 0 2 3	4 3 4 3 0	44.36 44.91 44.91 45.37 45.78

Chromium Chloride Hydrate, $CrCl_3 \cdot 6H_2O$ - (continued)

0			-0(0)
d(A)	I	hkl	2Θ(°)
1.949	8	- 1 3 3	46.56
1.940	25	3 3 1	46.79
1.936M	30	- 6 0 2	46.88
1.936M		0 0 6	46.88
1.9268	17	1 3 3	47.13
1.9047	6	4 2 3	47.71
1.9006	4	5 1 3	47.82
1.8824	8	-2 0 6	48.31
1.8748	7	3 1 5	48.52
1.8600	9	- 1 1 6	48.93
1.8547	8	3 3 2	49.08
1.8299	2	-4 2 4	49.79
1.8048	10	2 0 6	50.53
1.7893	7	- 3 3 3	51.00
1.7379M	5	3 3 3	52.62
1.7379M		4 2 4	52.62
1.7349	6	-3 1 6	52.72
1.7282	14	6 2 0	52.94
1.7084M	2	0 4 0	53.60
1.7084M		- 6 0 4	53.60
1.6907	6	0 4 1	54.21
1.6843+	5	0 2 6	54.43
1.6843+		- 6 2 2	54.43
1.6643+	5	-7 1 1	55.14
1.6643+		- 4 2 5	55.14
1.6454	3	3 1 6	55.83
1.6394	4	0 4 2	56.05
1.6266	7	5 3 1	56.53
1.6235M	7	2 4 1	56.65
1.6235M		- 1 3 5	56.65
1.6130	4	-1 1 7	57.05
1.5962M	3	2 2 6	57.71
1.5962M		6 0 4	57.71
1.5836	3	1 1 7	58.21
1.5762M	8	4 2 5	58.51
1.5762M		4 0 6	58.51
1.5711	12	7 1 2	58.72
1.5336M	3	- 3 1 7	60.30
1.5336M		- 3 3 5	60.30
1.5243M	6	- 5 1 6	60.71
1.5243M		-2 4 3	60.71
1.5103	4	- 4 2 6	61.33
1.5105	7		01.00

CAS registry no. 10101-53-8

Sample

The sample was prepared by heating $\mathrm{NH_4Cr(SO_4)_2}$ at 500 °C for 3 hours. The sample contained a very small percent of $\mathrm{Cr_2O_3}$.

Color

Reddish brown

Structure

Hexagonal, $R\bar{3}$ (148), Z = 6. [Kokkoros, 1965].

Lattice constants of this sample

a = 8.132(1) Ac = 21.943(6)

c/a = 2.6983

Volume

1256.8 A³

Density

(calculated) 3.109 g/cm³

Figure of merit

 $F_{30} = 40.0(0.014,55)$

Reference intensity

 $I/I_{corundum} = 1.55(5)$

Additional patterns

1. PDF card 18-393 [Kokkoros, 1965]

2. PDF card 18-394 [Watelle-Marion and Thiard, 1965]

References

Kokkoros, P. A. (1965). Mineral. Petrogr.

Mitt. 10, 45.

Watelle-Marion, G. and Thiard, R. (1965).

C. R. Acad. Sci. 261, 4105.

CuK $lpha_1$	$\lambda = 1.540598$	Ä;	temp	p.	25±1	°C
	nal standard	Si,	a =	5	. 43088	o A
d(Å)	I		hkl			2Θ(°)
5.93	50	0	1	2		14.93
4.327	45	1	0	4		20.51
4.070	15	1	1	0		21.82
3.658	25	0	0	6		24.31
3.555	100	1	1	3		25.03
2.965	35	0	2	4		30.11
2.721	40	1	1	6		32.89
2.644	11	2	1	1		33.88
2.395	9	2	1	4		37.52
2.347	11	3	0	0		38.31
2.274	3	1	2	5		39.59
2.235	8	3	0	3		40.32
2.163	9	2	0	8		41.72
2.092	6	1	1	9		43.20
2.029	3	2	1	7		44.61
1.975	4	3	0	6		45.91
1.923	5	3	1	2		47.23
1.909	5	1	2	8		47.59
1.8627	6	0		10		48.85
1.8395	4	1	3	4		49.51
1.7771	9	2	2	6		51.37
1.7390	3	0	4	2		52.58
1.6931	11	2		10		54.12
1.6573	4	1	3	7		55.39
1.6114	2	3	2	1		57.11
1.5981	3	2	3	2		57.63
1.5903	3	3	1	8		57.94
1.5613	2	2	2	9		59.12
1.5504	6	3	2	4		59.58
1.5366	6	4	1	0		60.17
1.5167	3	2	3	5		61.04
1.4818	3	0	4	8		62.64
1.4586	10	1		10		63.75
1.4425	4	3	0	12		64.55
L						

Sample
The hand separated sample is from U.S. National
Museum (NMNH R8105) from Mammoth Mine, Pinal
Co., AZ.

Major impurities
Approximately 10% PbSO₄ was present in this mineral as a second phase and was ignored.

Color Deep blue

Structure Monoclinic, $P2_1/m$ (11), Z=2. The structure was determined by Bachmann and Zeeman [1961]. Araki [1962] re-examined his earlier work and confirmed the above structure.

Lattice constants of this sample a = 9.6913(9)A b = 5.6503(6)

b = 5.6503(6)c = 4.6873(5) β = $102.66(1)^{\circ}$

a/b = 1.7152c/b = 0.8296

Volume 0 250.43 Å³

Density (calculated) 5.315 g/cm³

Figure of merit $F_{30} = 76.6(0.011,35)$

Additional patterns
1. PDF card 4-598 [Berry, 1951]

References
Araki, T. (1962). Mineral. J. Japan. 3, 282.
Bachmann, H.-G. and Zeeman, J. (1961). Acta
Crystallogr. 14, 747.
Berry. L. G. (1951). Amer. Mineral. 36, 512.

CuΚα ₁ λ =	= 1.540598	8 Å;	tem	р.	25±1	°C	
	standard	W, a	. =	3.1	6524	Å	
d(Å)	I		hkl			20(°)
9.46 4.849 4.731 4.521 3.805	11 40 3 60 9	1 1 2 -1 1	0 1 0 0 0	0 0 0 1 1		9. 18. 18. 19. 23.	74 62
3.717 3.625 3.556 3.151M 3.151M	3 30 55 100	-2 2 0 1 3	0 1 1 1 0	1 0 1 1 0		23. 24. 25. 28.	54 02 30
3.106 2.978 2.912 2.826 2.754	40 19 2 17 6	-2 2 -3 0 3	1 0 0 2 1	1 1 1 0 0		28. 29. 30. 31. 32.	98 68 64
2.707 2.587 2.424 2.405 2.365M	30 25 8 17 5	1 -3 2 0 3	2 1 2 2 0	0 1 0 1 1		33. 34. 37. 37. 38.	64 05 36
2.365M 2.344 2.317 2.267 2.261	4 20 20 20	4 -1 -4 1 -2	0 0 0 2 0	0 2 1 1 2		38. 38. 38. 39.	37 83 72
2.250 2.181M 2.181M 2.164 2.145	9 17 19 6	-2 3 4 -1 -4	2 1 1 1 1	1 1 0 2 1		40. 41. 41. 41. 42.	36 36 71
2.119M 2.119M 2.104 2.081 2.049	20 12 4 8	0 1 3 -3 2	1 0 2 0 2	2 2 0 2 1		42. 42. 42. 43. 44.	63 95 45
2.027 1.9021M 1.9021M 1.8469 1.8295	20 2 5 12	-3 2 -5 1 4	2 0 0 3 1	1 2 1 0 1		44. 47. 47. 49.	78 78 30
1.8128M 1.8128M 1.8018M 1.8018M 1.7932	20 17 14	3 4 2 -5 5	2 2 1 1 1	1 0 2 1 0		50. 50. 50. 50.	29 62 62
1.7769 1.7660M 1.7660M 1.7497 1.7416	7 9 5 8	0 -4 -2 2 0	2 1 2 3 3	2 2 2 0 1		51. 51. 51. 52. 52.	72 72 24

Copper Lead Hydroxide Sulfate, Linarite, $CuPb(OH)_2(SO_4)$ - (continued)

d(A)	I	hkl	2Θ(°)
1.6883	5	1 3 1	54.29
1.6803	8	- 2 3 1	54.57
1.6752	8	-3 2 2	54.75
1.6456	4	- 5 0 2	55.82
1.6264	5	5 0 1	56.54
1.6130	5	3 1 2	57.05
1.5804M	8	- 3 3 1	58.34
1.5804M		- 5 1 2	58.34
1.5765M	13	- 5 2 1	58.50
1.5765M		6 0 0	58.50
1.5718	9	5 2 0	58.69
1.5595	2	-1 0 3	59.20
1.5542M	2	-2 0 3	59.42
1.5542M		-4 2 2	59.42
1.5413	4	-6 1 1	59.97
1.5247	3	0 0 3	60.69
1.5079	4	-3 0 3	61.44
1.5033	4	-1 1 3	61.65
1.4891	6	4 0 2	62.30
1.4736M	4	3 3 1	63.03
1.4736M		4 3 0	63.03
1.4680	4	-1 3 2	63.30
1.4571	2	-3 1 3	63.83
1.4466	2	3 2 2	64.35
1.4216	2	-5 2 2	65.62
1.4124	6	0 4 0	66.10
1.4092+	6	5 2 1	66.27
1.4092+		-6 1 2	66.27
1.3878	2	-4 1 3	67.43
1.3802	3	-7 0 1	67.85
1.3763	4	6 2 0	68.07
1.3655M	3	2 0 3	68.68
1.3655M		-1 2 3	68.68
1.3576	2	6 1 1	69.14
1.3504	5	7 0 0	69.56
1.3490+	6	4 3 1	69.64
1.3490+		-1 4 1	69.64

CAS registry no. 456-22-4

Sample

The sample was NBS Standard Reference Material 2143.

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), Z = 4. The structure was qualitatively determined by Toussaint [1952].

Lattice constants of this sample

a = 26.545(4) A

b = 6.385(2)

c = 3.816(1)

 $\beta = 93.72(2)^{\circ}$

a/b = 4.1573

c/b = 0.5976

Volume 645.4 A³

Density

(calculated) 1.442 g/cm³

Figure of merit

 $F_{30} = 60.5(0.012,41)$

Reference intensity

 $I/I_{corundum} = 1.10(4)$

Additional pattern

 PDF card 11-730 [Institute of Physics, Cardiff, Wales]

Reference

Toussaint, J. (1952). Mem. Soc. Roy. Sci. Liege, Collect. 8, <u>12</u>, 1.

	CuKα ₁ λ	= 1.540598	A;	tem	р.	25±1 °C
	Internal	standard	Ag,	a =	4.	08651 Å
	d(A)	I		hkl		2Θ(°)
	13.26	85	2	0	0	6.66
	6.62	20	4	0	0	13.37
	6.21	6	1	1	0	14.26
	5.76	20	2	1	0	15.38
ı	5.178	100	3	1	0	17.11
ı						
	4.600	30	4	1	0	19.28
ı	4.412	2	6	0	0	20.11
	4.077	3	5	1	0	21.78
	3.805	5	-1	0	1	23.36
	3.737	10	1	0	1	23.79

d(Å)	I	hkl	2Θ(°)
3.580 3.312 3.274M 3.274M 3.226	75 35 70 65	-3 0 1 8 0 0 0 1 1 -1 1 1 1 1 1	24.85 26.90 27.22 27.22 27.63
3.194M 3.194M 3.172 3.134 3.005+	9 7 5 4	0 2 0 -5 0 1 1 2 0 2 1 1 3 2 0	27.91 27.91 28.11 28.46 29.71
3.005+ 2.940 2.875 2.856 2.715	8 5 4 4	5 0 1 8 1 0 4 2 0 -5 1 1 5 1 1	29.71 30.38 31.08 31.29 32.97
2.672 2.649 2.586 2.560 2.446+	5 2 5 3 4	9 1 0 10 0 0 6 2 0 6 1 1 10 1 0	33.51 33.81 34.66 35.02 36.71
2.446+ 2.423 2.404 2.395 2.299	5 4 4 7	0 2 1 -2 2 1 -9 0 1 -8 1 1 8 2 0	36.71 37.08 37.37 37.52 39.16
2.264M 2.264M 2.252M 2.252M 2.208	7 5 1L	8 1 1 4 2 1 11 1 0 -9 1 1 12 0 0	39.79 39.79 40.00 40.00 40.84
2.164 2.129 2.102M 2.102M 2.096M	1 2 4	9 2 0 9 1 1 6 2 1 2 3 0 -11 0 1	41.70 42.43 43.00 43.00 43.12
2.096M 2.087 2.039 2.007 1.942	2 1 1L 1	-7 2 1 12 1 0 10 2 0 -8 2 1 13 1 0	43.12 43.31 44.40 45.15 46.75
1.921M 1.921M 1.892 1.847M 1.847M	1 1 3	11 2 0 -9 2 1 14 0 0 -2 3 1 -13 0 1	47.28 47.28 48.06 49.31 49.31
1.844 1.825 1.815M 1.815M	3 6 2	9 2 1 0 1 2 12 2 0 14 1 0	49.38 49.93 50.24 50.24

CAS registry no. 10294-29-8

Sample

The sample was prepared by dissolving Au metal in aqua regia. The dark red intermediate crystals obtained were dried at 200 °C for one hour. The AuCl crystals were found to be metastable, disproportionately decomposing into Au metal and Au₂Cl₆ [Janssen et al., 1974]. Au₂Cl₆ was not detected in this sample; however, the Au metal present was used as the internal standard.

Color Yellow

Structure

Tetragonal, $I4_1/amd$ (141), Z=8. The structure was studied by Janssen et al. [1974]. The structure had been reported to be orthorhombic by Capella and Schwab [1965].

Lattice constants of this sample

 $a = 6.7425(9) \stackrel{\circ}{A}$ c = 8.694(1)

c/a = 1.2894

Volume o 395.2 A³

Density

(calculated) 7.812 g/cm³

Figure of merit $F_{16} = 81.8(0.010,20)$

Additional patterns

1. PDF card 27-241 [Janssen et al., 1974]

2. Capella and Schwab [1965]

References

Capella, L. and Schwab, C. (1965). C. R. Acad. Sci. 260, 4337.

Janssen, E. M. W., Folmer, J. C. W., and Wiegers, G. A. (1974). J. Less-Common Metals 38, 71.

$CuK\alpha_1$	$\lambda = 1.540598$	3 Å;	temp	٥.	25±1	°C
	nal standard	Au,	a =	4	.0786	o A
d(A)	I		hkl			2Θ(°)
5.327	100	1	0	1		16.63
3.371	4	2	0	0		26.42
3.213	5	1	1	2		27.74
2.849	60	2	1	1		31.37
2.664M	100	2	0	2		33.62
2.664M		1	0	3		33.62
2.384	25	2	2	0		37.71
2.173	18	0	0	4		41.52
2.089	30	2	1	3		43.27
1.8278M	14	3	2	1		49.85
1.8278M		2	0	4		49.85
1.7760	4	3	0	3		51.41
1.6846M	20	4	0	0		54.42
1.6846M		1	0	5		54.42
1.6063M	17	4	1	1		57.31
1.6063M		2	2	4		57.31
1.5711M	10	4	0	2		58.72
1.5711M		3	2			58.72
1.5061	4	2	1	3 5		61.52
1.4245M	20	4	2	2		65.47
1.4245M		4	1	3		65.47
1.3754	4	3	0	5		68.12

Iron Phosphate Hydrate (Vivianite), Fe₃(PO₄)₂·8H₂O

Sample

The sample was made by slow reaction of $\rm H_3PO_4$ on $\rm FeSO_4$ solution with some $\rm H_2SO_4$ added. The flask was freed of air by flushing with natural gas and left with occasional shaking for two weeks.

Color

Grayish purplish blue

Structure

Monoclinic, I2/m (12), Z = 2 [Barth, 1937]. The structure was determined by Mori and Ito [1950]. It is isostructural with Fe₃(AsO₄)₂·8H₂O (parasymplesite) [Ritz et al., 1974].

Lattice constants of this sample

a = 10.034(3) Å

b = 13.449(3)

c = 4.707(2) $\beta = 102.65(3)^{\circ}$

a/b = 0.7461

c/b = 0.3500

Volume 619.7 Å³

Density

(calculated) 2.688 g/cm³

Figure of merit

 $F_{30} = 52.6 (0.015,38)$

Polymorphism

A polymorph of $Fe_3(PO_4)_2 \cdot 8H_2O$ occurs naturally, is triclinic and is called metavivianite [Ritz et al., 1974].

Additional pattern

1. PDF card 3-70 [Dow Chemical Co., Midland, MI]

References

Barth, T. F. W. (1937). Amer. Mineral. <u>22</u>, 325.

Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.

Ritz, C., Essene, E. J., and Peacor, D. R. (1974). Amer. Mineral. <u>59</u>, 896.

CuKα ₁ λ	= 1.540598	3 Å;	tem	p. 2	25±1 °C
Internal	standard	Si,	a =	5.4	43088 Å
d(A)	Ι		hkl		2Θ(°)
7.93 6.73 4.900 4.558 4.341	13 100 12 5 2	2	2 0 0	0	11.15 13.15 18.09 19.46 20.44

d(A)	I	hkl	2Θ(°)
4.081 3.849 3.768 3.361 3.343	12 7 1L 1 2	1 0 -1 2 0 4	0 21.76 1 23.09 1 23.59 0 26.50 1 26.64
3.210 2.985 2.960 2.770 2.728	16 10 8 4 9	-3 0 2 1 2 4	1 27.77 1 29.91 1 30.17 0 32.29 1 32.80
2.706 2.637 2.593 2.530 2.514	9 6 4 8 3	3 3	1 33.08 0 33.97 0 34.57 1 35.45 1 35.68
2.448 2.421 2.321 2.296 2.279M	1 6 7 1	3 0 0 5 0 0	0 36.68 1 37.11 1 38.77 2 39.20 2 39.51
2.279M 2.233 2.194 2.173 2.108M	5 5 2 1	3 2 -3 4 -2 5 0 2 1 1	1 39.51 1 40.35 1 41.11 2 41.53 2 42.86
2.108M 2.075 2.039 2.012M 2.012M	4 1L 2		1 42.86 0 43.59 0 44.40 1 45.03 1 45.03
1.964M 1.964M 1.936M 1.936M 1.886M	2 2 2	1 6	1 46.19 1 46.19 0 46.89 1 46.89 0 48.22
1.886M 1.816 1.793 1.786 1.772	2 1 3 2	-5 2 4 3 -3 6 -4 5 0 7	1 48.22 1 50.20 1 50.89 1 51.10 1 51.52
1.6809 1.6599 1.5974M 1.5974M 1.5834	6 2 3	-3 5 4 5 3 3	0 54.55 2 55.30 1 57.66 2 57.66 0 58.22
1.5404	1	1 8	1 60.01

CAS registry no. 10028-22-5

Sample

The sample was made by heating $Fe_2(SO_4)_3$ *XH₂O at 200 °C for several hours, followed by heating at 500 °C in a sealed glass tube for 1 hour.

Color

Yellow white

Structure

Hexagonal, $R\overline{3}$ (148), Z = 6 [Kokkoros, 1965].

Lattice constants of this sample

a = 8.236(1)Ac = 22.166(6)

c/a = 2.6914

Volume o

1302.1 Å³

Density (calculated) 3.060 g/cm³

Figure of Merit $F_{30} = 32.8(0.017,53)$

Reference intensity
I/I corundum = 2.26(11)

Additional pattern
1. PDF card 18-652 [Kokkoros, 1965]

Reference

Kokkoros, P. A. (1965). Tschermak's Mineral. Petrogr. Mitt. 10, 45.

CuK α_1	λ = 1.540598	o A;	ten	ıp.	25±1	°C
	nal standard	Si,	a =	5	. 43088	3 Å
d(A)	I		hk£			2Θ(°)
6.01	50	0	1	2		14.72
4.380	45	1	0	4		20.26
4.124	13	1	1	0		21.53
3.699	7	0	0	6		24.04
3.599	100	1	1	3		24.72
3.002	40	0	2	4		29.74
2.751	45	1	1	6		32.52
2.678	10	2	1	1		33.43
2.581	1	0	1	8		34.73
2.426	9	2	1	4		37.03
2.378	12	3	0	0		37.80
2.301	1	1	2	5		39.11
2.263	7	3	0	3		39.80
2.190	2	2	0	8		41.19
2.114	7	1	1	9		42.74
2.054	3	2	1	7		44.06
1.999	4	3	0	6		45.33
1.947	3	3	1	2		46.62
1.931	4	1	2	8		47.01
1.882	6	0	2	10		48.31
1.863	6	1	3	4		48.85
1.847	1	0	0	12		49.31
1.799	11	2	2	6		50.71
1.760	3	0	4	2		51.90
1.7123	11	2	1	10		53.47
1.6781	4	1	3	7		54.65
1.6330	1	3	2	1		56.29
1.6099	5	3	1	8		57.17
1.5794	1	2	2	9		58.38
1.5694	7	3	2	4		58.79
1.5561	7	4	1	0		59.34
1.5346	2	2	3	5		60.26
1.5231	2	4	1	3		60.76
1.4995	2	0	4	8		61.82
1.4757	7	1	3	10		62.93

CAS registry no. 16651-91-5
Sample The sample was prepared by making a saturated aqueous solution of fresh recrystallized PbBr ₂ . To this was added a 10% solution of NaOH. The precipitate was left for 80 hours in the liquid to promote growth of the crystals.
Color Colorless
Structure Orthorhombic, Pnam (62), Z = 4. The structure of PbBr(OH) was determined by Møller [1966]. PbBr(OH) is isostructural with SbBrS and PbCl(OH).
Lattice constants of this sample
a = 7.3850(8)A $b = 10.013(1)$ $c = 4.0835(5)$
a/b = 0.7375 c/b = 0.4078
Volume 301.96 A ³
Density (calculated) 6.689 g/cm ³
Figure of merit F ₃₀ = 78.7(0.012,31)
Reference Intensity I/I corundum = 5.9(3)
Additional patterns 1. PDF card 6-257 [Shell Petroleum Co., Ltd.] 2. Møller [1966]
Reference Møller, C. K. (1966). Kgl. Dan. Vidensk. Sels. Mat. Fys. Medd. <u>35</u> , 15.

CuKα ₁ λ	. = 1.540598	8 Å;	temp	p .	25±1 °C
	l standard	Si,	a =	5 .	.43088 A
d(A)	I		hkl		2Θ(°)
5.93 4.998 4.139 3.781 3.693	9 9 55 4 10	1 0 1 0 2	1 2 2 1 0	0 0 0 1	14.93 17.73 21.45 23.51 24.08
3.462 3.363 3.042 2.970 2.908	25 100 12 20 45	2 1 1 2 1	1 1 3 2 2	0 1 0 0 1	25.71 26.48 29.34 30.06 30.72
2.737 2.641 2.584 2.504 2.475	4 40 50 6 10	2 2 0 0 2	0 1 3 4 3	1 1 1 0 0	32.69 33.91 34.69 35.83 36.26
2.439 2.403 2.391 2.371 2.210	3 18 25 20 15	1 2 3 1 3	3 2 1 4 2	1 1 0 0 0	36.82 37.40 37.59 37.92 40.80
2.118 2.072 2.064 2.043 1.982	19 4 6 20 2	2 2 3 0 3	3 4 1 0 3	1 0 1 2 0	42.65 43.64 43.83 44.31 45.75
1.943 1.933 1.8901 1.8483 1.8313	14 8 2 4 12	3 1 0 2 1	2 5 2 4 2	1 0 2 1 2	46.70 46.97 48.10 49.26 49.75
1.7975 1.7860 1.7824 1.7597M 1.7597M	8 6 5 7	0 2 3 2 2	5 0 3 5 1	1 2 1 0 2	50.75 51.10 51.21 51.92 51.92
1.7475 1.6959 1.6823M 1.6823M 1.6688	13 4 25 3	1 1 2 4 0	5 3 2 0 6	1 2 2 1 0	52.31 54.03 54.50 54.50 54.98
1.6151 1.6120 1.5944 1.5824 1.5757	19 20 2 4 5	4 3 4 0 2	3 4 2 4 3	0 1 1 2 2	56.97 57.09 57.78 58.26 58.53
1.5531M 1.5531M 1.5476 1.5211 1.5123	16 14 7 1	3 3 1 2 1	5 1 4 6 6	0 2 2 0 1	59.47 59.47 59.70 60.85 61.24

Lead Bromide Hydroxide, PbBr(OH) - (continued)

d(Å)	I	hkl	2Θ(°)
1.4998	7	3 2 2	61.81
1.4610	4	5 1 0	63.64
1.4518	7	3 5 1	64.09
1.4251	7	3 5 1 2 6 1	65.44
1.4166	3	5 2 0	65.88
	_		
1.4036M	4	1 7 0	66.57
1.4036M		1 5 2	66.57
1.3967	3	4 4 1	66.94
1.3811	1	3 6 0	67.80
1.3692	1	4 0 2	68.47
11005	-		551.,
1.3574M	2	4 5 0	69.15
1.3574M	_	4 1 2	69.15
1.3499	3	0 7 1	69.59
1.3385	5	5 2 1	70.27
1.3276	9	1 7 1	70.93
	-		, , , , ,
1.2929	4	1 2 3	73.14
1.2820	2	5 3 1	73.86
1.2669M	10	4 3 2	74.89
1.2669M		2 1 3	74.89
1.2603	6	0 3 3	75.35
			, 5 . 33
1.2513	1	0 8 0	75.99
1.2426	1	1 3 3	76.62
1.2197	6		78.33
1.2146	5	2 6 2 5 4 1	78.72
1.1928	3	2 3 3	80.45
	_		
1.1885M	5	5 5 0	80.80
1.1885M		5 1 2	80.80

Sample The sample is holotype material from U.S. National Museum (NMNH #135815). The locality of this sample can be stated only in general terms. The crystals occur as detritus in the soils near Antsirabe in Madagascar, and a specific site for the occurrence of the type mineral is not known [Dunn et al., 1977].
Color Dark olive brown
<pre>Optical data Uniaxial(-), N = 1.637, N = 1.621 [Dunn et al., 1977].</pre>
Structure Hexagonal, R3m (160), Z = 3, isostructural with tourmalines [Dunn et al., 1977].
Lattice constants of this sample a = 15.847(1) Å c = 7.1080(7)
c/a = 0.4485
Volume o 1546.0 A ³
Density (calculated) 3.06 g/cm^3 [based on $\text{Ca}(\text{Li}_{1.74}\text{Al}_{1.26})\text{Al}_6\text{B}_3\text{Si}_6\text{O}_2\text{7}\cdot\text{52}(\text{OH})_2\cdot\text{48}(\text{F,OH})$ according to empirical formula by Dunn et al. (1977)].
Figure of merit $F_{30} = 62.0(0.015,32)$
Reference Dunn, P. J., Appleman, D. E., and Nelen, J. E. (1977). Amer. Mineral. 62, 1121.

CuKα ₁ λ	= 1.540598	A;	tem	p. 2	5±1	°C
	standard	W, a	=	3.16	524	o A
d(Å)	I		hkl			2Θ(°)
7.94	5	1	1	0		11.14
6.33 4.943	6 30	1 0	0 2	1 1		13.99 17.93
4.581	19	3	0	0		19.36
4.197	50	2	1	1		21.15
3.962	55	2	2	0		22.42
3.445	50	0	1	2		25.84
3.357	25	1 4	3	1 1		26.53 28.84
3.093 2.995	9 30	4	0	0		29.81
2.933	100			. 2		30.45
2.881	9	1 3	2	1		31.02
2.641	2	3	3	0		33.92
2.598	14	3	1	2		34.49
2.559	85	0	5	1		35.04
2.468	1	0	4	2		36.37
2.437	4	2	4	1		36.85
2.368	18	0 2	0	3		37.96
2.356 2.328	15 24	5	3 1	2		38.17 38.65
2.288 2.270	5 4	6 1	0	0 3		39.34 39.67
2.173	7	5	0	2		41.53
2.151	17	4	3	1		41.96
2.105	19	3	0	3		42.94
2.095	19	4	2	2		43.15
2.033	30	2	2	3		44.53
2.025 2.008	40 6	1 1	5 6	2 1		44.71 45.12
1.980	5	4	4	0		45.78
1.9054	· 35	3	4	2		47.69
1.8901	3	3	5	1		48.10
1.8582	5 7	4	1	3		48.98
1.8375		6	2	1		49.57
1.8031	3	6	1	2		50.58
1.7619	10	1	0	4		51.85
1.7200	1	0	2	4		53.21
1.7061 1.6812	2 2	5 2	4	1 4		53.68
1.6781	3	2	6	2		54.65
1.6459	17	6	0	3		55.81
1.6319	14	2	7	1		56.33
1.6112	2	5	2	3		57.12
1.5851	13	5	5	0		58.15
1.5782	8	4	0	4		58.43
1.5750	6	4	5	2		58.56
1.5670	3	8 3	1	1		58.89
1.5479 1.5371	3 4	3 4	2 6	4		59.69 60.15
1.5247	6	9	0	ō		60.69

Lithium Calcium Aluminum Boron Hydroxy Silicate, Liddicoatite, $Ca(Li,Al)_3Al_6B_3Si_6O_{27}(0,OH)_3(OH,F)$ - (continued)

d(Å)	I	hk.	l	20(°)
1.5161	6	7 2	2	61.07
1.4974	4	8 2	0	61.92
1.4913	14	0 5	4	62.20
1.4655	6	2 4		63.42
1.4414	20	5 1	4	64.61
1.4226	3	7 4		65.57
1.4139	5	0 1	_	66.02
1.4102	7	1 9	1	66.22
1.3958M	17	6 3	3	66.99
1.3958M		4 3	4	66.99
1.3713	1	1 2	5	68.35
1.3475	8	10 0	1	69.73
1.3334	2	5 6		70.58
1.3208	4	6 6		71.35
1.3167M	8	5 5	3	71.61
1.3167M		3 5	4	71.61
1.3134	8	0 4	5	71.82
1.3022	10	10 1	0	72.53
1.2987	7	6 2	4	72.76
1.2926	2	5 7	1	73.16
1.2826	2	9 0	3	73.82
1.2760	2	8 4		74.27
1.2690	4	9 3		74.75
1.2656	5	8 2	3	74.98
1.2622	12	5 0		75.22
1.2496	5	5 4	4	76.11
1.2463	5 3	4 2		76.35
1.2316	3	1 5		77.43
1.2316	3 3	1 5		77.43
1.2289	4	0 11		77.63

Sample

The sample was made by slow evaporation at room temperature of an aqueous solution of Li_2CrO_4 .

Color

Strong orange yellow

Structure

Orthorhombic, $P2_12_12_1$ (19), Z = 4. The cell was obtained from the axial ratios of Groth [1908] assuming a density near 2.1 and a Z = 4.

Lattice constants of this sample

a = 7.746(1) A

b = 12.011(2)

c = 5.5094(7)

a/b = 0.6449

c/b = 0.4587

Volume 512.56 Å³

Density

(calculated) 2.150 g/cm³

Figure of merit

 $\bar{F}_{30} = 74.6(0.012,35)$

Additional pattern

1. PDF card 1-819 [Hanawalt et al., 1938]

Reference

Groth, P. (1908). Chemische Krystallographie II, (Wilhelm Engelmann, Leipzig, Germany) p. 365.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

$CuK\alpha_1\lambda =$	1.540598	A; t	emp	. 25	5±1 °C
Internal	standard	Si,	a =	5.4	3088 Å
d(A)	I		hkl		2Θ(°)
6.52	25	1	1	0	13.57
5.012	25	0	1	1	17.68
4.751	90	1	2	0	18.66
4.489	85	1	0	1	19.76
4.205	75	1	1	1	21.11
4.061	85	0	2	1	21.87
3.687	60	2	1	0	24.12
3.593	25	1	2	1	24.76
3.558	60	1	3	0	25.01
3.239	4	0	3	1	27.52
3.170	70	2	0	1	28.13
3.062	100	2	1	1	29.14
3.002	75	0	4	Ô	29.74
2.993	75	1	3	1	29.83
2.802M	11	2	2	î	31.91

d(A)	I	hkl	2Θ(°)
	1	nkx	20(*)
2.802M	20	1 4 0	31.91
2.784 2.754	20	2 3 0 0 0 2	32.13
2.754	80 12	0 0 2 0 1 2	32.48 33.34
2.597	3	1 0 2	34.51
2.397	3	1 0 2	34.31
2.537	7	1 1 2	35.35
2.525	7	3 1 0	35.52
2.494	25	1 4 1	35.98
2.485	45	2 3 1	36.12
2.382	19	1 2 2	37.74
2.373M	40	2 4 0	37.89
2.373M		3 2 0	37.89
2.338	25	3 0 1	38.48
2.293M	5	1 5 0	39.25
2.293M		3 1 1	39.25
2.271	3	0 3 2	39.66
2.245	4	2 0 2	40.14
2.206	14	2 1 2	40.88
2.179M	45	2 4 1	41.40
2.179M		3 2 1	41.40
0 170	17	2 2 0	/1 50
2.170	17	3 3 0	41.59
2.118	12	1 5 1	42.65
2.103	13	2 2 2 2 2 5 0	42.98
2.041	16	2 5 0 0 4 2	44.34
2.029	10	0 4 2	44.62
2.018	11	3 3 1	44.87
1.9586M	5	2 3 2	46.32
1.9586M		3 4 0	46.32
1.9365	8	4 0 0	46.88
1.9134	20	2 5 1	47.48
1.8839	9	3 0 2	48.27
1.8614	5	3 1 2	48.89
1.8424	4	4 2 0	49.43
1.8271M	4	4 0 1	49.87
1.8271M		1 6 1	49.87
1.8149	12	0 1 3	50.23
1.8149	10	4 1 1	50.49
1.7988	5	2 4 2	50.71
1.7863	7	1 0 3	51.09
1.7676	9	1 1 3	51.67
	•	, ,	
1.7481	2	4 2 1	52.29
1.7135	1	1 2 3	53.43
1.6755M	9	3 5 1	54.74
1.6755M	25	1 7 0 2 0 3	54.74
1.6591	25	2 0 3	55.33
1.6435	6	2 1 3	55.90
1.6272	20	4 4 0	56.51
1.6030	3	1 7 1	57.44
1.5962	7	3 4 2	57.71
1.5824	3	3 6 0	58.26
1.5708	4	4 1 2	58.73
1.5700	7	, 1 2	30.73

CAS registry no. 12188-25-9

Sample

The sample was prepared by heating $\text{Li}_2\text{C}_2\text{O}_4$ and SnO_2 at 800 °C for 10 minutes followed by 950 °C for 20 minutes.

Color

Colorless

Structure

Monoclinic, A2/a (15), Z = 8, [Scheer et al., 1955; Lang, 1954]. The structure of Li_2SnO_3 has been studied by Kreuzburg et al. [1970].

Lattice constants of this sample

a = 10.027(2) A

b = 9.181(2)

c = 5.301(2)

 $\beta = 100.26(2)^{\circ}$

a/b = 1.0921c/b = 0.5774

Volume o 480.1 Å³

Density

(calculated) 4.996 g/cm³

Figure of merit

 $F_{30} = 27.9(0.014,80)$

Reference intensity
I/I corundum = 4.1(3)

Polymorphism

There is a second form of Li₂SnO₃ which differs in its stacking [Lang, 1966].

References

Kreuzburg, G., Stewner, F., and Hoppe, R. (1970).
Z. Anorg. Allg. Chem. 379, 242.
Lang, G. (1954). Z. Anorg. Allg. Chem. 276, 77.
Lang, G. (1966). Z. Anorg. Allg. Chem. 348, 246.
Scheer, J. J., Van Arkel, A. E., and Heyding,

R. D. (1955). Can. J. Chem. 33, 683.

$CuK\alpha_1 \lambda =$	1.540598	8 A;	tem	р.	25±1 °C
Internal	standard	Ag,	a =	4.	08651 Å
d(Å)	I		hkl		20(°)
4.932 4.586 4.539 4.386 4.166	100 17 10 7 3	2 0 0 -1 1	0 2 1 1 2	0 0 1 1 0	17.97 19.34 19.54 20.23 21.31
3.899 3.630 3.106 2.886 2.673	2 2 1 1 2	1 -2 2 -3 3	1 1 1 1 2	1 1 1 1 0	22.79 24.50 28.72 30.96 33.50
2.641 2.608M 2.608M 2.495M 2.495M	1 55 25	0 -1 0 -2 1	3 0 0 3	1 1 2 2 1	33.92 34.36 34.36 35.97 35.97
2.466 2.324 2.293 2.288 2.154M	9 1 3 2 65	4 -4 0 -1 -3	0 1 4 2 3	0 1 0 2 1	36.40 38.72 39.25 39.34 41.91
2.154M 1.974 1.7343 1.7321M 1.7321M	20 3 3	2 3 -1 -1 0	0 3 1 4 5	2 1 3 2 1	41.91 45.94 52.74 52.81 52.81
1.7233M 1.7233M 1.6527 1.6446 1.6180	2 12 6 1	-1 0 -5 6 -5	5 4 3 0 2	1 2 1 0 2	53.10 53.10 55.56 55.86 56.86
1.5300M 1.5300M 1.5164 1.4612M 1.4612M	19 17 15	0 -1 5 2 1	6 3 3 6 3	0 3 1 0 3	60.46 60.46 61.06 63.63 63.63
1.3202M 1.3202M 1.3041M 1.3041M 1.3002	6 5 7	-2 0 -6 0 4	0 6 1 0 6	4 2 3 4 0	71.39 71.39 72.41 72.41 72.66
1.2921 1.2723M 1.2723M 1.2685M 1.2685M	3 2 1	-7 0 -1 -2 -1	3 7 2 2 7	1 1 4 4 1	73.19 74.52 74.52 74.78 74.78
1.2473 1.2325 1.2093 1.2081M 1.2081M	9 3 3 3	2 1 5 2 4	6 5 6 0 3	2 3 0 4 3	76.28 77.36 79.13 79.23 79.23
1.1990 1.1459M 1.1459M 1.1224	4 1L 4	7 8 -5 4	3 1 6 6	1 1 2 2	79.95 84.48 84.48 86.68

CAS registry no. 14567-64-7	C
	1
Sample A sample of MgSO ₄ ·7H ₂ O was obtained from	d(A
Fisher Scientific Co. of Fairlawn, NJ. The material was heated first at 150 °C, then sealed in a tube and heated for 1 3/4 hours at 400 °C.	4.8 3.4 3.3 3.3
Color Colorless	3.1
Structure Monoclinic, A2/a (15), Z = 4. The structure was determined by Leonhardt and Weiss [1957] and confirmed by Bregeault et al. [1972].	3.0 2.5 2.5 2.4 2.3
Lattice constants of this sample $ \begin{array}{lll} a = & 7.5110(9) & \mathring{A} \\ b = & 7.611(1) \\ c = & 6.921(1) \\ \beta = & 116.17(1)^{\circ} \end{array} $	2.3 2.1 2.0 2.0 2.0
a/b = 0.9868 c/b = 0.9093 Volume 355.1 A^3	1.9 1.9 1.9 1.8
Density (calculated) 2.589 g/cm ³ Figure of merit F ₃₀ = 60.5(0.011,47)	1.8 1.7 1.7 1.7
Reference intensity I/I = 1.02(4)	1.6 1.6
Additional pattern 1. PDF card 13-102 [Kubisz, 1960] (natural mineral)	1.6
References Bregeault, JM., Herpin, P., and Coing-Boyat, J. (1972). Bull. Soc. Chim. Fr. 1972, 2247. Kubisz, J. (1960). Bull. Acad. Pol. Sci. Ser. Sci. Geol. Geogr. 8, 101.	1.5 1.5 1.5
Sci. Geol. Geogr. <u>8</u> , 101. Leonhardt, H. J. and Weiss, R. (1957). Naturwis- senschaften <u>44</u> , 338.	1.5

CuKα ₁ λ	= 1.540598	ßÄ;	tem	٥.	25±1	°C	
Interna	l standard	Si,	a =	5	.43088	3 A	
d(Å)	I		hkl			20((°)
4.815	75	0	1	1		18.	
3.405	100	1	1	1		26.	
3.351	70	-2	1	1		26.	
3.313	70	1	2	0		26.	
3.106	13	0	0	2		28.	.72
3.051	40	-2	0	2		29.	
2.560	35	-1	2	2		35	
2.523	30	2	2	0		35	
2.401	3	2	1	1		37.	
2.380	3	-2	2	2		37	. 76
2.342	4	-1	3	1		38	
2.185	7	-1	1	3		41.	
2.099	9	-2	3	1		43.	
2.054	20	1	2	2		44.	
2.023	3	-3	2	2		44.	. / /
1.965	8	-3	1	3		46.	
1.934	4	3	2	0			.94
1.9039M	5	2	0	2		47	
1.9039M		0	4	0		47	
1.8657	1	-4	0	2		48	. //
1.8125	3	3	1	1			.30
1.7919M	1	-4	1	1		50	.92
1.7919M		2	3	1			. 92
1.7288M	1L	-2	0	4		52	
1.7288M		1	1	3		52	.92
1.7029	3	2	2	2		53	
1.6750	14	-4	2	2		54	
1.6577	5	2	4	0		55	
1.6227	8	0	4	2		56	
1.6043	3	0	3	3		57	.39
1.5866	7	-3	3	3		58	
1.5531	4	0	0	4			. 47
1.5401M	2	4	2	0			.02
1.5401M		-1	2	4			.02
1.5265	2	- 3	2	4		60	. 61
1.5030	4	3	3	1		61.	.66
1.4524M	3	1	3	3			.06
1.4524M		3	4	0			. 06
1.4366	2	-5	1	3		64	. 85
1.4160	2	-4	2	4		65	.91
1.3975	1	- 5	2	2		66	.90

Sample The sample was prepared by heating a 3:2 molar mixture of ${\rm MnCO_3}$ and ${\rm (NH_4)_2HPO_4}$ overnight at 850 °C.

Color Pinkish white

Structure

Monoclinic, P2₁/c (14), Z = 4. The cell was found by use of the Visser program [1969] and by comparison with β -Zn₃(PO₄)₂ and Cd₃(PO₄)₂. The space group was assigned by consideration of the absences in the powder pattern.

Lattice constants of this sample

a = 8.446(2) A b = 10.059(3) c = 8.047(2) $\beta = 114.27(2)^{\circ}$

a/b = 0.8396c/b = 0.8000

Volume 623.2 Å³

Density (calculated) 3.781 g/cm^3 (assuming Z = 4)

Figures of merit $F_{30} = 54.0(0.013,44)$ $M_{20} = 31.1$

Polymorphism

 $\mathrm{Mn_3(PO_4)_2}$ is also reported to crystallize in a graftonite structure [Calvo, 1968]. Stephens and Calvo [1969] also describe a second monoclinic form of $\mathrm{Mn_3(PO_4)_2}$ which they call " β ".

Additional pattern

 PDF card 3-0465 [Dow Chemical Co., Midland, MI]

References

89.

Calvo, C. (1968). Amer. Mineral. $\underline{53}$, 742. Stephens, J. S. and Calvo, C. (1969). Can. Chem. $\underline{47}$, 2215. Visser, \overline{J} . W. (1969). J. Appl. Crystallogr. $\underline{2}$,

 $CuK_1 \lambda = 1.540598 \stackrel{\circ}{A}$; temp. $25\pm 1 \stackrel{\circ}{\circ} C$ Internal standard W, $a = 3.16524 \stackrel{\circ}{A}$

		,			-0
d(Å)	I		hkl		2Θ(°)
6.10 5.92 4.207 4.010 3.852	8 6 35 16 7	1 0 1 -1 2	1 1 2 0 0	0 1 0 2 0	14.50 14.96 21.10 22.15 23.07
3.726 3.669 3.597 3.458 3.446	55 10 12 25 13	-1 0 2 -2 0	1 0 1 0	2 2 0 2 2	23.86 24.24 24.73 25.74 25.83
3.341 3.269 3.218 3.135 3.073	35 90 100 30 65	1 -2 -2 -1 1	2 1 2 2 3	1 2 1 2 0	26.66 27.26 27.70 28.45 29.03
3.018 2.963 2.882 2.849 2.827	25 45 60 20 55	-1 0 1 -2 2	3 2 0 2 1	1 2 2 2 1	29.58 30.14 31.01 31.37 31.62
2.772 2.705 2.681M 2.681M 2.616	10 9 4	1 -3 1 -3 -2	1 1 3 0 3	2 1 1 2 1	32.27 33.09 33.40 33.40 34.25
2.593 2.573 2.528 2.489 2.453	25 25 60 2 14	-3 -1 2 3 -3	1 3 3 1 2	2 2 0 0 1	34.57 34.84 35.48 36.06 36.60
2.408 2.375 2.368 2.357 2.315	8 20 18 18	-2 0 -3 -1 -2	3 1 2 2 2	2 3 2 3 3	37.31 37.85 37.97 38.15 38.87
2.285 2.248 2.215 2.184M 2.184M	2 4 5 5	3 -3 2 2 1	2 1 3 1 3	0 3 1 2 2	39.41 40.08 40.71 41.30 41.30
2.157 2.132 2.095+ 2.095+ 2.089	6 3 5	-2 -1 -4 -3 -1	4 4 0 3 3	1 2 2 2 3	41.85 42.37 43.15 43.15 43.28
2.052M 2.052M 2.034 2.006 1.986	15 11 2 2	-4 1 -2 -2 3	1 1 4 0 2	2 3 2 4 1	44.09 44.09 44.50 45.16 45.64

Manganese Phosphate, $\mathrm{Mn_3(PO_4)_2}$ - (continued)

d(A)	I	h	ıkl		2Θ(°)
1.975M	7	0	3	3	45.92
1.975M		-1	0	4	45.92
1.968	11	-2	1	4	46.08
1.940M	13	-1	1	4	46.80
1.940M		0	5	1	46.80
1.933+	17	1	2	3	46.96
1.933+		-4	2	2	46.96
1.916	20	-4	1	3	47.40
1.891	6	4	1	0	48.09
1.874M	8	-3	4	1	48.53
1.874M		-3	1	4	48.53
1.860	16	2	3	2	48.93
1.835M	9	-3	4	2	49.64
1.835M		1	5	1	49.64

Sample

A sample of MnSO₄ was obtained from J. T. Baker Co., Phillipsburg, NJ. Crystals were formed from a saturated solution of the material at room temperature. The crystals slowly changed to the monohydrate when left in open air and were finally heated at 250 °C for 2½ hours.

Color

Colorless

Structure

Monoclinic, A2/a (15), Z = 4, isostructural with $CoSO_4 \cdot H_2O$. The structure was determined by Le Fur et al. [1966].

Lattice constants of this sample

a = 7.766(1) A

b = 7.666(1)

c = 7.120(1) $\beta = 115.85(1)$ °

a/b = 1.0130

c/b = 0.9288

Volume 381.5 A³

Density

(calculated) 2.943 g/cm³

Figure of merit

 $F_{30} = 77.8(0.010,37)$

Reference intensity

 $I/I_{corundum} = 1.91(7)$

Additional pattern

1. PDF card 14-166 [Pistorius, 1961]

References

Le Fur, Y., Coing-Boyat, J., and Bassi, G. (1966). C. R. Acad. Sci. Ser. C 262, 632. Pistorius, C. W. F. T. (1961). Z. Anorg. Allg. Chem. 302, 226.

$CuK\alpha_1 \lambda =$	1.54059	8 Å;	temp	.	25±1 °C
Internal	standard	Ag,	a =	4.	08651 Å
d(A)	I		hkl		2Θ(°)
4.916	50	0	1	1	18.03
4.855	30	- 1	1	1	18.26
3.834	8	0	2	0	23.18
3.507	100	1	1	1	25.38
3.445	20	-2	1	1	25.84
3.361	30	1	2	0	26.50
3.203	1L	0	0	2	27.83
3.139	40	-2	0	2	28.41
2.606	15	-1	2	2	34.38
2.580	30	2	2	0	34.74
					3

d(A)	I	hkl	2Θ(°)
		, n	
2.483	1	2 1 1	36.15
2.457	1	0 2 2	36.54
2.446	3	-3 1 1	36.71
2.366	7	-1 3 1	38.00
2.245	10	- 1 1 3	40.13
2.1/5		1 2 1	/2.00
2.145	6	1 3 1	42.09
2.131	2	-2 3 1	42.38
2.109	7	1 2 2	42.85
2.072	1	-3 2 2	43.65
2.0193	8	- 3 1 3	44.85
1.9894	1	3 2 0	45.56
1.9722	4	2 0 2	45.98
1.9164	2	0 4 0	47.40
1.8762	4	3 1 1	48.48
1.8536	1L	-4 1 1	49.11
1.0330	11	4 1 1	49.11
1.8316	1L	2 3 1	49.74
1.8159	1L	-3 3 1	50.20
1.7795	1	-2 0 4	51.30
1.7528	4	2 2 2	52.14
1.7472	2	4 0 0	52.32
1.7291	2	- 1 3 3	52.91
1.7218M	8	-4 2 2	53.15
1.7218M		- 2 3 3	53.15
1.6806	3	2 4 0	54.56
1.6443	5	0 4 2	55.87
1 6200	2	0 2 2	E 6 07
1.6389	3	0 3 3	56.07
1.6193	5	-3 3 3	56.81
1.6149	4	-2 2 4	56.98
1.6015	3	0 0 4	57.50
1.5896	1L	4 2 0	57.97
1.5809	1	-1 2 4	58.32
1.5701	1	-4 0 4	58.76
1.5658	1L	-3 2 4	58.94
1.5432	3	3 3 1	59.89
1.5128	1L	-3 4 2	61.22
1.3120	11	-5 4 2	01.22
1.4961	1L	4 1 1	61.98
1.4887M	2	- 1 5 1	62.32
1.4887M		1 3 3	62.32
1.4810M	3	-5 1 1	62.68
1.4810M		- 5 1 3	62.68
1 /770	•	0 0 1	(0.00
1.4778	2	0 2 4	62.83
1.4643M	1L	-4 3 3	63.48
1.4643M		3 2 2	63.48
1.4526	1L	-4 2 4	64.05
1.4390	1L	-5 2 2	64.73
1.4290	1L	1 5 1	65.24

Sample
The sample was obtained from Alfa Division,
Ventron Corp., Danvers, MA.

Color Yellowish white

Structure

Orthorhombic, $P2_1mn$ (31), Z=2. The structure was determined by Bonefačić [1963] and Kokkoros and Rentzeperis [1963]. Aurivillius [1964] reports that the symmetry is monoclinic rather than orthorhombic.

Lattice constants of this sample

a = 4.8150(2) Å b = 6.5752(3)

c = 4.7810(2)

a/b = 0.7323

c/b = 0.7271

Volume 0 151.36 Å³

Density (calculated) 6.509 g/cm³

Figure of merit F₃₀ = 118(0.008,31)

Additional patterns

 PDF card 13-519 [Kokkoros and Rentzeperis, U. Thessaloniki, Greece]

2. Aurivillius and Malmros [1961]

References

Aurivillius, K. (1964). Ark. Kemi 24, 151. Aurivillius, K. and Malmros, B. (1961). Acta Chem. Scand. 15, 1932.

Bonefačić, A. $(\overline{19}63)$. Croat. Chem. Acta $\underline{35}$, 195.

Kokkoros, P. A. and Rentzeperis, P. J. (1963). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 119, 234. CuK α_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

internal	standard	w, a	=	3.16524	Α
 d(Å)	I		hkl		2Θ(°)
4.782	12	0	0	1	18.54
3.884	85	1	1	0	22.88
3.865	85	0	1	1	22.99
3.392	100	1	0	1	26.25
3.288	75	0	2	0	27.10
3.014	45	1	1	1	29.62
2.707	4	0	2	1	33.06
2.408	25	2	0	0	37.32
2.390	17	0	0	2	37.60
2.361	60	1	2	1	38.09
0.04		_	_	•	
2.2457	20	0	1	2	40.12
2.1509	10	2	0	1	41.97
2.1412	20	1	0	2	42.17
2.0431	35	2	1	1	44.30
2.0361	25	1	1	2	44.46
1.9936M	35	1	3	0	45.46
1.9936M		0	3	1	45.46
1.9423	25	2	2	0	46.73
1.9333	16	0	2	2	46.96
1.8406	12	1	3	1	49.48
1.7988	8	2	2	1	50.71
1.7939	14	1	2	2	50.86
1.6967	7	2	0	2	54.00
1.6440	17	0	4	0	55.88
1.6154	7	0	3	2	56.96
1.5936	3	0	0	3	57.81
1.5593	5	3	1	0	59.21
1.5545	4	0	4	1	59.41
1.5353	9	2	3	1	60.23
1.5313	8	1	3	2	60.40
1.5215	6	3	0	1	60.83
1.5128	1L	1	0	3	61.22
1.5077	5	2	2	2	61.45
1.4791	15	1	4	1	62.77
1.4743	19	1	1	3	63.00
1.4342	3	0	2	3	64.97
1.3807	10	3	2	1	67.82
1.3576	5	2	4	0	69.14
1.3541	5	ō	4	2	69.34
1.3415	5	2	3	2	70.09
110.15	J		Ū	_	
1.3329	1	3	0	2	70.61
1.3293	3	2	0	3	70.83
1.3060M	4	3	1	2	72.29
1.3060M		2	4	1	72.29
1.3039	5	1	4	2	72.42
1.2950	1	3	3	0	73.00
1.2684M	4	1	5	0	74.79
1.2684M		ō	5	1	74.79
1.2502	1	3	3	î	76.07
1.2452	5	1	3	3	76.43

Mercury Sulfate, $HgSO_4$ - (continued)

d(Å)	I	hkl	2Θ(°)
1.2348	2	3 2 2	77.19
1.2320	4	2 2 3	77.40
1.2261	2	1 5 1	77.84
1.2035	1	4 0 0	79.59
	2	2 4 2	
1.1804	2	2 4 2	81.47
1.1758	3	0 1 4	81.86
1.1673	1L	4 0 1	82.58
1.1601	2	1 0 4	83.21
1.1522	2	0 5 2	83.91
1.1442	1	0 4 3	84.63
1.1442	1	0 4 3	84.03
1.1387	1	3 3 2	85.14
1.1302	1	4 2 0	85.93
1.1218	2	2 5 1	86.73
1.1206	1	1 5 2	86.85
1.1166	4	3 4 · 1	87.24
1.1100	_	J 4 1	07.24
1.1144	4	3 1 3	87.45
1.1002	1L	4 2 1	88.88
1.0960	2	0 6 0	89.31
1.0940	2	1 2 4	89.52
1.0751	1L	4 0 2	91.53
1.0751	12	4 0 Z	71.55
1.0681	1L	0 6 1	92.30
1.0611	1	4 1 2	93.09
1.0566	2	2 1 4	93.61
1.0493	2	0 3 4	94.46
1.0430	3	1 6 1	95.22
1.0430	3	1 0 1	93.22
1.0394	3	2 5 2	95.65
1.0352	1	3 4 2	96.16
1.0335	2	2 4 3	96.37
1.0302	1	4 3 1	96.78
1.0254	1L	1 3 4	97.39
		,	,,,,,
1.0218	2	4 2 2	97.85
1.0171	1L	3 5 0	98.46
1.0050	3	3 3 3	100.08
.9974	2	2 6 0	101.13
.9949	2	3 5 1	101.47
.,,,,		J J 1	2021.7
.9924	3	1 5 3	101.83

Sample The sample was reagent material obtained from Kahlbaum, Berlin, Germany. Color Yellowish white Structure Monoclinic, P2/a (13), Z = 2, isostructural with mercury selenate. The structure was determined by Dorm [1969]. Lattice constants of this sample a = 8.365(1) Ab = 4.4262(5)c = 6.2785(9) $\beta = 91.77(1)^{\circ}$ a/b = 1.8899c/b = 1.4185Volume 232.34 Å³ Density (calculated) 7.108 g/cm^3 Figure of merit $F_{30} = 76.4(0.013,30)$ Reference intensity $I/I_{corundum} = 3.4(3)$ Additional pattern 1. PDF card 1-0838 [Hanawalt et al., 1938] References Dorm, E. (1969). Acta Chem. Scand. <u>23</u>, 1607. Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuKα ₁ λ =	= 1.540598	3 Å; t	emp.	25±1 °C
Internal	standard	W, a	= 3.	16524 Å
d(Å)	I	h	kl	2Θ(°)
6.28 4.427 4.182 3.916 3.619	4 80 75 1 25	0 2 1	0 1 1 0 0 0 1 0 1 1	14.08 20.04 21.23 22.69 24.58
3.530 3.432 3.342 3.296 3.136	4 25 7 13 20	2 -1 1	0 1 0 1 1 1 1 1 0 2	25.21 25.94 26.65 27.03 28.44
3.039 2.712 2.560 2.549 2.473	100 12 25 20 7	2 0 -2	1 0 1 1 1 2 0 2 0 2	29.37 33.00 35.02 35.18 36.29
2.468 2.433 2.359 2.228 2.214	7 1L 2 2 12	3 -3	1 2 1 2 1 0 1 1 2 0	36.38 36.92 38.12 40.46 40.72
2.209 2.189 2.159 2.139 2.090M	20 2 6 1L 20		1 2 1 1 1 2 2 0 0 0	40.82 41.21 41.81 42.22 43.25
2.090M 2.087 2.029 2.021 2.002	14 6 5 1L	0 0 -1 1 -4	0 3 2 1 2 1 2 1 0 1	43.32
1.964 1.956 1.8909M 1.8909M 1.8759	4 7 16 1	4 2 0 4 -2	0 1 2 0 1 3 1 0 2 1	46.38 48.08 48.08
1.8600 1.8561 1.8487 1.8085 1.7958	5 4 6 4 6	2 -1 2 0 4	2 1 1 3 0 3 2 2 1 1	49.04 49.25 50.42
1.7747 1.7644 1.7613 1.7413 1.7333	1 6 5 5	-1 -4 1 -2 3	2 2 0 2 2 2 1 3 2 0	51.77 51.87 52.51
1.7159 1.7055 1.6784 1.6705 1.6626	1 6 2 4 2	4 2 -3 -2 3	0 2 1 3 2 1 2 2 2 1	53.70 54.64 54.92

Mercury Sulfate, Hg_2SO_4 - (continued)

1.6386 6 -4 1 2 56.0 1.5992 1L 4 1 2 57.5 1.5684 1L 0 0 4 58.8 1.5643 1L 5 1 0 59.0 1.5286 1 -5 1 1 60.5 1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4838M -4 2 1 62.5 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4174 3 -1 3 1 65.8 1.4174 3 -1 3 1)	2Θ(°)		hkl		I	d(Å)
1.5992 1L 4 1 2 57.5 1.5684 1L 0 0 4 58.8 1.5643 1L 5 1 0 59.0 1.5286 1 -5 1 1 60.5 1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4753 1L 0 3 0 62.9 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4174 3 -1 3 1 65.8 1.4174 3 -1 3 1 66.0	9	55.69	2	2	2	2	1.6492
1.5992 1L 4 1 2 57.5 1.5684 1L 0 0 4 58.8 1.5643 1L 5 1 0 59.0 1.5286 1 -5 1 1 60.5 1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4753 1L 0 3 0 62.9 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4174 3 -1 3 1 65.8 1.4174 3 -1 3 1 66.0	8	56.08	2	1	-4	6	1.6386
1.5684 1L 0 0 4 58.8 1.5643 1L 5 1 0 59.0 1.5286 1 -5 1 1 60.5 1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 66.0	9	57.59		1	4	1L	1.5992
1.5286 1 -5 1 1 60.5 1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	3	58.83		0	0	1L	1.5684
1.5188 4 4 2 0 60.9 1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	0	59.00	0	1	5	1L	1.5643
1.5044 1 3 2 2 61.6 1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	2	60.52	1	1	~5	1	1.5286
1.4893 1L 1 2 3 62.2 1.4838M 1L -2 0 4 62.5 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	5	60.95	0			4	1.5188
1.4838M 1L -2 0 4 62.5 1.4838M -4 2 1 62.5 1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	0	61.60	2		3	1	1.5044
1.4838M	9	62.29	3	2	1	1L	1.4893
1.4753 1L 0 3 0 62.9 1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	5	62.55	4	0	-2	1L	1.4838M
1.4692 1 4 2 1 63.2 1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	5	62.55	1	2	-4		1.4838M
1.4561 1 4 0 3 63.8 1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	5	62.95	0	3	0	1L	1.4753
1.4390 1 -2 2 3 64.7 1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	4	63.24	1	2	4	1	1.4692
1.4358 1 0 3 1 64.8 1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	8	63.88		0	4	1	1.4561
1.4222 1 -4 1 3 65.5 1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	3	64.73	3	2	-2	1	1.4390
1.4174 3 -1 3 1 65.8 1.4138 2 1 3 1 66.0	9	64.89	1	3	0	1	1.4358
1.4138 2 1 3 1 66.0	9	65.59	3	1	-4	1	1.4222
	4	65.84	1	3	- 1	3	1.4174
1.4070 1 -2 1 4 66.3	3	66.03	1	3	1	2	1.4138
	9	66.39	4	1	-2	1	1.4070
1.3910 1 2 3 0 67.2	5	67.25	0	3	2	1	1.3910
1.3831 2 4 1 3 67.6	9	67.69	3	1	4	2	1.3831
	7	67.87		2	-4	2	1.3798

Synonym 1. 3-Pyridinecarboxylic Acid
CAS registry no. 59-67-6
Sample The sample was NBS Standard Reference Material 148. It is used for checking microdeter- minations of carbon, hydrogen and nitrogen.
Color Colorless
Optical data Biaxial(-), $N_{\alpha} = 1.424(2)$, $N_{\beta} = 1.717$, $N_{\gamma} \sim 1.79$. $2V = 46^{\circ}$ [Wright and King, 1950].
Structure Monoclinic, $P2_1/a$ (14), $Z = 4$, [Wright and King, 1950].
Lattice constants of this sample
a = $7.222(2)$ Å b = $11.672(3)$ c = $7.178(2)$ $\beta = 113.42(2)$ °
a/b = 0.6187 c/b = 0.6150
Volume o 555.3 A ³
Density (calculated) 1.473 g/cm ³
Figure of merit $F_{30} = 47.8(0.011,57)$
Reference intensity I/I = 0.95(3)
Additional pattern 1. PDF card 24-1843 [Wright and King, 1950]
Reference Wright, W. B. and King, G. S. D. (1950). Acta Crystallogr. 3, 31.

CuKα ₁ λ =	= 1.54059	8 A; temp. 25±	to °C
Internal	standard	W, a = 3.1652	24 Å
d(A)	I	hkl	2Θ(°)
5.73 4.362 4.185 3.743 3.588	100 40 25 7 55	0 1 1 0 2 1 -1 2 1 1 1 1 -2 0 1	15.45 20.34 21.21 23.75 24.79
3.429 3.314 3.271M 3.271M 3.188	70 80 20 50	-2 1 1 2 0 0 1 2 1 -1 3 1 2 1 0	25.96 26.88 27.24 27.24 27.96
3.053 3.043 2.916M 2.916M 2.881	7 8 3	-2 2 1 -1 2 2 0 4 0 -2 1 2 2 2 0	29.23 29.32 30.63 30.63 31.01
2.869 2.773 2.670M 2.670M 2.628M	3 4 4	0 2 2 1 3 1 1 4 0 0 4 1 -1 3 2	31.15 32.26 33.54 33.54 34.09
2.628M 2.513 2.381 2.347 2.298	6 5 12 5	-1 4 1 0 3 2 -2 3 2 1 4 1 -2 0 3	34.09 35.70 37.75 38.31 39.16
2.259 2.196 2.178 2.157 2.145M	7 11 10 3 3	-1 4 2 0 0 3 -1 5 1 0 1 3 -3 2 2	39.87 41.07 41.43 41.85 42.09
2.145M 2.009 1.984 1.977M	3 2 2	1 3 2 1 5 1 -3 3 2 -3 1 3 2 0 2	42.09 45.08 45.68 45.86 45.86
1.956 1.949 1.928 1.905 1.866M	2 1 1 1	-2 5 1 2 1 2 1 4 2 0 5 2 1 6 0	46.37 46.56 47.09 47.71 48.77
1.866M 1.8496M 1.8496M 1.8094 1.8064	1 3 4	0 6 1 -1 6 1 1 1 3 -3 4 2 -2 4 3	48.77 49.22 49.22 50.39 50.48
1.7833+ 1.7833+ 1.7628+ 1.7628+	7 3	1 2 3 -2 0 4 -4 1 1 2 3 2	51.18 51.18 51.82 51.82

Synonym

1. Ethanedioic acid dihydrate

2. Hydrogen oxalate hydrate

CAS registry no. 6153-56-6

Sample

Oxalic acid hydrate, analytical reagent was obtained from Mallinkrodt, St. Louis, MO 63147. It was dissolved in distilled water at room temperature. The solution was allowed to evaporate partly at room temperature and the precipitate was filtered.

Color Colorless

Structure

Monoclinic, $P2_1/a$ (14), Z = 2. The structure was last refined by Ahmed and Cruickshank [1953] who correlated various earlier data.

Lattice constants of this sample

a = 11.890(3) Å

b = 3.6070(7)c = 6.121(1)

 $\beta = 103.31(3)^{\circ}$

a/b = 3.2966c/b = 1.6971

Volume o 255.4 Å³

Density (calculated) 1.639 g/cm³

Figure of merit $F_{30} = 52.8(0.012,47)$

Additional pattern

 PDF card 14-832 [de Wolff, Techn. Phys. Dienst, Delft, Holland]

Reference intensity
I/I = 1.63(6)

Reference

Ahmed, F. R. and Cruickshank, D. W. J. (1953). Acta Crystallogr. 6, 385.

CuKα ₁	$\lambda = 1.540598$	8 A;	temj	. o	25±1	°C	
Intern	al standard	Si,	a =	5	. 43088	o A	
d(Å)	Ι		hkl			20((°)
5.94	25	0	0	1		14.	
5.79	4	2	0	0		15.	
4.729	30	-2	0	1		18.	
3.737 3.443	1L 16	2	0 1	1		23.	
3.443			1	U		25.	00
3.075	100	-1	1	1		29.	
2.937	10	-2	0	2		30.	
2.874	8	~4	0	1		31.	
2.632	1 4	3	1	0		34.	
2.595	4	2	1	1		34.	33
2.562	4	-3	1	1		34.	
2.431 2.396	17 6	2 4	0	2		36. 37.	
2.364	12	-4	0	2		38.	
2.333	2	-1	1	2		38.	
2.296	6	0	1	2		39.	20
2.279M	12	3	1	1		39.	
2.279M		-2	1	2		39.	
2.257	8	4	1	0		39.	
2.178	1	1	1	2		41.	42
1.986	3	0	0	3		45.	65
1.978	3	-4	1	2		45.	
1.947	1L	5	1	0		46.	
1.929	2	6	0	0		47.	
1.8354	2	3	1	2		49.	63
1.8210	1L	-6	0	2		50.	
1.8035	1L	0	2	0		50.	
1.7734	2 1	-1 -2	1 1	3		51.	
1.7578	1 1L	2	0	3		51. 51.	
1.7395	1	0	1	3		52.	
1.7236	2	-1		1		53.	
1.7218+	2	6	0	1		53.	
1.7218+	1L	2 6	2 1	0		53. 53.	
}		U					
1.6915	1L	1	2	1		54.	
1.6710	2	1	1	3		54.	
1.6446	1	-4	1	3		55.	
1.6169	1 1	-3	2	1		56.	
1.3602	1	2	1	3		58.	. 55
1.5422	2	0	2	2		59.	
1.5371M	3	3	2	1		60.	
1.5371M	2	-2	2	2		60.	
1.5307M	2	4	2	0		60.	
1.5307M		-2	0	4		60.	43

Synonym 1. 2,4,6-Trinitcophenol
CAS registry no. 88-89-1
Sample The sample was obtained from the General Chemical Division, Allied Chemical and Dye Corp., New York, NY. It was recrystallized from water.
Color Light yellow
Structure Orthorhombic, P2 ₁ ca (29), Z = 8 [Bredig and Möller, 1929].
Lattice constants of this sample
$a = 9.723(4)\mathring{A}$ b = 19.139(6) c = 9.271(3)
a/b = 0.5080 c/b = 0.4844
Volume ° 1725.3 Å ³
Density (calculated) 1.764 g/cm ³
Figure of merit $F_{30} = 42.5(0.017,41)$
Additional pattern 1. PDF card 9-789 [Morse and Baun, Wright Air Development Center, Wright-Patterson AFB, Ohio]
Reference Bredig, M. A. and Möller, H. (1929). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 71, 331.

CuKa ₁	$\lambda = 1.540598$	8 A;	temp	.	25±1 °C
	enal standard	Ag,	a =	4.	.08651 Å
d(A)	I		hkl		2Θ(°)
9.56 6.65 6.38 6.34 5.49	20 3 6 6 45	0 0 0 1 1	2 2 3 1 2	0 1 0 1	9.24 13.31 13.88 13.96 16.13
5.245 4.784 4.706 4.629M 4.629M	1 40 15 25	0 0 2 0 1	3 4 1 0 3	1 0 0 2 1	16.89 18.53 18.84 19.16 19.16
4.507 4.327 4.247 4.184 4.087	11 16 19 20 19	0 2 0 1 1	1 2 4 0 1	2 0 1 2	19.68 20.51 20.90 21.22 21.73
3.901 3.869 3.831M 3.831M 3.750	90 100 60 70	1 2 1 0 0	4 3 2 5 3	1 0 2 0 2	22.78 22.97 23.20 23.20 23.71
3.569 3.500 3.411 3.351 3.326M	30 45 19 14 12	2 1 2 2 0	3 3 4 0 4	1 2 0 2 2	24.93 25.43 26.10 26.58 26.78
3.326M 3.203 3.191 3.152 3.015	4 5 13 90	1 2 0 1 0	5 4 6 4 6	1 0 2 1	26.78 27.83 27.94 28.29 29.61
2.954 2.944 2.909 2.879 2.862	7 9 7 25 40	0 0 1 1 2	5 2 1 6 5	2 3 3 1 1	30.23 30.34 30.71 31.04 31.23
2.822 2.815 2.780 2.673 2.667	9 13 6 25 27	1 1 0 1 2	5 2 3 3 6	2 3 3 0	31.68 31.76 32.17 33.50 33.57
2.626 2.597 2.576 2.564 2.532	8 9 11 11 6	0 0 3 2 1	6 4 4 6 7	2 3 1 1 1	34.11 34.51 34.80 34.96 35.42
2.523 2.509 2.411 2.389 2.355M	5 9 3 3 5	2 1 4 3 4	4 1 5	2 3 0 1 0	35.76 37.27 37.62

Picric Acid, $C_6H_3N_3O_7$ - (continued)

d(Å) I hkl 20(°)	
2 2554 0 7 2 30 10	
2.355M 0 7 2 38.18	
2.313 8 2 6 2 38.90	
2.313 8 2 6 2 38.90 2.290M 2 2 4 3 39.32	
2.290M 1 7 2 39.32	
2.273 2 4 3 0 39.62	
2.255M 3 1 0 4 39.94	
2.255M 1 8 1 39.94	
2.208M 3 3 6 1 40.83	
2.208M 4 3 1 40.83	
2.180M 2 0 3 4 41.39	
2.180M 3 2 3 41.39	
2.153 3 4 0 2 41.93	
2.126M 9 0 8 2 42.49	
2.126M 1 3 4 42.49	
2.094 3 2 0 4 43.17	
2.085 4 0 4 4 43.36	
2.076 5 1 8 2 43.56	
2.041+ 5 3 6 2 44.35	
2.041+ 4 3 2 44.35	
2.021 4 2 6 3 44.82	
2.004M 3 1 7 3 45.22	
2.004M 4 5 1 45.22	
1.948M 4 2 9 0 46.58	
1.948M 2 8 2 46.58	
1.948M 2 8 2 46.58 1.931 3 3 5 3 47.02	

CAS registry no. 10141-00-1

Sample

The sample was prepared by heating $KCr(SO_4)_2 \cdot 12H_2O$ at 300 °C for several days. The crystallinity was improved by heating at 700 °C. However some impurity lines developed at this temperature, and therefore there may be minor errors in the intensities.

Color

Medium yellow green

Structure

Hexagonal, P321 (150), Z = 1, isostructural with other dehydrated alums such as $KA1(SO_4)_2$ and $NH_4A1(SO_4)_2$. The structure of these compounds was studied by Vegard and Maurstad [1928].

Lattice constants of this sample

a = 4.7547(6)A c = 8.054(2)

c/a = 1.6939

Volume 0 157.68 Å³

Density

(calculated) 2.983 g/cm³

Figure of merit

 $F_{19} = 74.6(0.010,25)$

Additional pattern

1. PDF card 3-325 [Dow Chemical Co.]

Reference

Vegard L. and Maurstad, A. (1928). Z. Kristallogr, Kristallgeometrie Kristallphys. Kristallchem. 69, 519.

CuK $lpha_1$	$\lambda = 1.540598$	Ă;	tem	ρ.	25±1	°C
	nal standard S	Si,	a =	5	. 43088	s Å
d(Å)	τ		hkl			2Θ(°)
8.06	40	0	0	1	_	10.97
4.115	15	1	0	0		21.58
3.664	100	1	0	1		24.27
2.879	75	1	0	2		31.04
2.685	10	0	0	3		33.34
2.377	35	1	1	0		37.81
2.280	8	1	1	1		39.50
2.0466	10	1	1	2		44.22
1.9948	4	2	0	1		45.43
1.8333	19	2	0	2		49.69
1.8085	13	1	0	4		50.42
1.7795	1	1	1	3		51.30
1.6110	2	ō	ō	5		57.13
1.5566	3	2	1	0		59.32
1.5364	10	1	1	4		60.18
1.5288	8	2	1	1		60.51
1.4514	13	2	1	2		64.11
1.4398	4	2	0	4		64.69
1.3724	12	3	0	0		68.29

CAS registry no. 13718-65-5

Sample

The sample was precipitated by adding ethyl alcohol to a concentrated solution of KOH and $Fe(OH)_3$ in H_2SO_4 .

Color

Colorless

Structure

Monoclinic, C2/m (12), Z = 2, [Hutton, 1959].

Lattice constants of this sample

a = 8.155(1)A

b = 5.1539(6)

c = 7.877(1)

 $\beta = 94.85(1)^{\circ}$

a/b = 1.5823

c/b = 1.5284

Volume o 329.9 Å³

Density

(calculated) 2.890 g/cm³

Figure of merit

 $F_{30} = 56.2(0.017,32)$

Reference intensity

 $I/I_{corundum} = 0.99(3)$

Additional patterns

1. PDF card 12-632 [Hutton, 1959]

2. Corey and Sidhu [1945]

References

Hutton, C. O. (1959). Amer. Mineral. 44, 1105. Corey, R. C. and Sidhu, S. S. (1945). J. Am. Chem. Soc. 67, 1490.

$CuK\alpha_1 \lambda =$	1.540598	8 A;	temp	p.	25±1 °C
Internal	standard	Si,	a =	5	.43088 A
d(Å)	I		hkl		2Θ(°)
7.87 4.354 4.066 3.885 3.739M	70 11 50 70 65	0 1 2 -1 -2	0 1 0 1 0	1 0 0 1 1	11.23 20.38 21.84 22.87 23.78
3.739M 3.494 2.985 2.854 2.711	55 100 50 6	1 2 -1 1 2	1 0 1 1 0	1 1 2 2 2	23.78 25.47 29.91 31.32 33.02
2.617 2.578 2.449 2.399 2.343	6 30 1 55 2	0 0 0 3 -3	0 2 2 1 1	3 0 1 0 1	34.24 34.77 36.67 37.46 38.39
2.288M 2.288M 2.197 2.176 2.154	10 3 1 13	-2 -1 1 2 0	0 1 1 2 2	3 3 0 2	39.34 39.34 41.04 41.46 41.91
2.120M 2.120M 2.073 2.031 2.007	18 2 7 1	-2 2 2 4 -4	2 0 2 0 0	1 3 1 0 1	42.61 42.61 43.63 44.57 45.13
1.980 1.963 1.941 1.927 1.869M	2 3 13 3 12	3 0 -2 4 -4	1 0 2 0 0	2 4 2 1 2	45.79 46.22 46.77 47.13 48.69
1.869M 1.837M 1.837M 1.829 1.821	10 14 6	2 -3 0 -2 -1	2 1 2 0 1	2 3 3 4 4	48.69 49.58 49.58 49.81 50.05
1.7597 1.7450 1.7111M 1.7111M 1.7055	6 11 4 3	1 4 -2 2 3	1 0 2 0 1	4 2 3 4 3	51.92 52.39 53.51 53.51 53.70
1.6801 1.6492 1.5836 1.5691 1.5609	2 5 2 4 4	1 -1 -4 0	3 3 2 0 2	0 1 1 5 4	54.58 55.69 58.21 58.80 59.14
1.5552 1.5500 1.5353 1.5137 1.4974M	8 8 4 12 5	-1 5 1 -4 5	3 1 3 2 1	2 0 2 2 1	59.38 59.60 60.23 61.18 61.92

Potassium Iron Sulfate (Yavapaiite), $KFe(SO_4)_2$ - (continued)

d(Å)	I	hkl	,	2Θ(°)
1.4913	9	-2 2	4	62.20
1.4827	2	- 5 1	2	62.60
1.4657	6	3 1	4	63.41
1.4510	9	3 1 3 3	0	64.13
1.4453	10	4 2	2	64.41
1.4251+	2	2 2	4	65.44
1.4251+		-1 3	3	65.44
1.4036M	5	-4 2	3	66.57
1.4036M		5 1	2	66.57
1.3538M	2	6 0	0	69.36
1.3538M		-6 0	1	69.36
1.3234	3	4 2	3	71.19
1.3078	2	0 0	6	72.17
1.2936	1	-3 3	3	73.09
1.2885M	6	5 1	3	73.43
1.2885M		0 4	0	73.43
1.2682	6	-1 1	6	74.80
1.2669	9	- 5 1	4	74.89
1.2281	1	2 4	0	77.69
1.2184	1	-2 4	1	78.43
1.2157	4	2 0	6	78.64
1.2086	2 2	2 4	1	79.19
1.1990M	2	6 2	0	79.95
1.1990M		- 6 2	1	79.95
L				

These data are essentially the same pattern reported by Swanson et al. [1963], with minor revisions. The pattern has been indexed using crystallographic data published since 1963. The very small sample used then was a special preparation and is no longer available. The original sample had been prepared from a mixture of a soluble ruthenium salt with KCl and concentrated HNO3.
Color Very dark red
Optical data Biaxial(+), N_{α} = 1.750, N_{β} = 1.762, N_{γ} = 1.777, 2V \sim 90°
Structure Orthorhombic, Pmnb (62), Z = 4 [Khodeshova and Bokii, 1964; de Wolff, 1968].
Lattice constants of this sample
a = 10.369(4)A b = 13.296(4) c = 6.894(3)
a/b = 0.7798 c/b = 0.5185
Volume 950.4 Å ³
Density (calculated) 2.701 g/cm ³
Figure of merit $F_{30} = 54.6(0.018,31)$
Additional patterns 1. PDF card 24-886, revised by PDF editors [Swanson et al., 1963] 2. Powder Diffraction Data, [1976]. The data is very nearly the same as that given here.
References Khodeshova, T. S. and Bokii, G. B. (1964). J. Struct. Chem. 5, 130. Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 387. Swanson, H. E., Morris, M. C., Stinchfield, R. P., and Evans, E. H. (1963). Nat. Bur. Stand. U.S. Monogr. 25, Sec. 2, 29. de Wolff, P. M. (1968). J. Appl. Crystallogr. 1, 108.

CuKα ₁ λ =	= 1.540598	3 Å; t	em	25±	1 °C
	standard	Ag, a	. =	4.08	651 Å
d(Å)	I	ŀ	ıkl		20(°)
6.13	8	0 1	1	1	14.44 15.40
5.75 5.61	100 95	1	2	0	15.79
5.28	17	1	1	1	16.78
5.19	25	2	0	0	17.06
4.790	30	0	2	1	18.51
4.352 4.085	1L 6	1 2	2	1 0	20.39 21.74
3.962	10	2	1	1	22.42
3.731	4	0	3	1	23.83
3.520	25	2	2	1	25.28
3.509 3.450	25 25	1 0	3	1 2	25.36 25.80
3.335	16	0	1	2	26.71
3.325	16	0	4	0	26.79
3.176	1L	1	1	2	28.07
3.091 3.068	12 11	3 3	0	1	28.86 29.08
3.028	15	2	3	1	29.48
2.996	14	0	4	1	29.80
2.934	7	1	2	2	30.44
2.879	13	1 2	4 0	1 2	31.04 31.13
2.871 2.805	13 35	2	1	2	31.13
2.800M	35	3	2	1	31.94
2.800M		2	4	0	31.94
2.720 2.632M	35 8	0 2	3	2	32.90 34.03
2.632M	O	1	3	2	34.03
2.594M	50	2	4	1	34.55
2.594M		4	0	0	34.55
2.481	1L 7	0 2	5 3	1 2	36.18 37.29
2.409 2.393	10	0	4	2	37.29
2.277	15	4	2	1	39.54
2.262	10	3	4	1	39.82
2.238 2.211	4 10	2 1	5 1	1 3	40.26 40.78
2.167	10 1L	1	6	0	41.65
2.137	1L	3	3	2	42.26
2.105	7	0	5	2	42.93
2.072 2.063	14 16	4	0 5	2 2	43.66 43.84
2.047	6	4	1	2	44.22
2.037	7	2	6	0	44.44
2.000	4	1	3	3	45.30
1.980 1.959	10 4	5 4	2	0 1	45.78 46.32
1.954	4	2	6	1	46.44

CAS registry no. 506-64-9

Sample

The sample was precipitated by adding AgNO₃ solution to one of KCNS.

Color

Colorless

Structure

Monoclinic, C2/c (15), Z = 8, [Lindqvist, 1957].

Lattice constants of this sample

 $a = 8.774(2) \stackrel{\circ}{A}$ b = 7.972(1) c = 8.182(2)

 $\beta = 93.78(2)^{\circ}$

a/b = 1.1006

c/b = 1.0263

Volume o 571.1 A³

Density

(calculated) 3.860 g/cm³

Figure of merit

 $F_{30} = 54.6(0.014,39)$

Reference intensity

 $I/I_{corundum} = 2.95(9)$

Additional pattern

1. PDF card 12-382 [Pistorius, University of California, Los Angeles, Calif.]

Reference

Lindqvist, J. (1957). Acta Crystallogr. 10, 29.

	CuKα ₁ λ :	= 1.540598	3 Ă;	tem	р.	25±1	°C
	Internal	standard	Si,	A =	5.	43088	o A
	d(A)	I		hkl			2Θ(°)
	5.890	65	1	1	0		15.03
i	4.674	100	1	1	1		18.97
	4.079	5	0	0	2		21.77
	3.577	25	0	2	1		24.87
	3.426	3	-1	1	2		25.99

d(A)	I	hkl		2Θ(°)
3.089 2.945 2.891 2.850 2.810	55 10 12 9 19	-2 0 2 2 2 0 0 2 -2 2	2 0 2 2 1	28.88 30.33 30.91 31.36 31.82
2.732 2.648 2.542 2.512 2.430	80 10 14 13 4	2 2 -3 1 1 3 -1 1 1 1	1 1 0 3 3	32.75 33.82 35.28 35.71 36.97
2.415 2.341 2.247 2.214 2.188	4 17 25 13 6	1 3 2 2 0 2 3 1 4 0	1 2 3 2 0	37.20 38.42 40.09 40.72 41.22
2.177 2.140 2.046 2.041 1.993M	13 4 4 13 2	-1 3 1 3 -2 2 0 0 -3 1	2 2 3 4 3	41.44 42.20 44.23 44.35 45.47
1.993M 1.965 1.9361 1.9191 1.9036	2 4 4 11	0 4 3 3 0 4 4 2 1 1	0 0 1 0 4	45.47 46.15 46.89 47.33 47.74
1.8991 1.8920M 1.8920M 1.8777 1.8737	11 12 12 8	-2 0 -4 2 3 3 4 0 3 1	4 1 1 2 3	47.86 48.05 48.05 48.44 48.55
1.8145 1.8051 1.7916 1.7818 1.7607	3 5 4 4 2	2 4 2 0 0 4 -2 4 2 4	0 4 2 1	50.24 50.52 50.93 51.23 51.89
1.7401 1.7105 1.6747 1.6527 1.6405	6 1 2 3 5	3 3 5 1 -2 4 5 1 2 4	2 0 2 1 2	52.55 53.53 54.77 55.56 56.01
1.6125 1.6084 1.5772 1.5441M	2 3 2 2	-4 2 0 4 1 3 -4 0 -1 5	3 3 4 4 1	57.07 57.23 58.47 59.85 59.85
1.5373 1.5275 1.4736 1.4618M 1.4618M	3 4 3 4	1 5 4 2 4 4 5 3 -4 4	1 3 0 0	60.14 60.57 63.03 63.60 63.60
	2.945 2.891 2.850 2.810 2.732 2.648 2.542 2.512 2.430 2.415 2.341 2.247 2.140 2.148 2.177 2.140 2.046 2.041 1.993M 1.993M 1.993M 1.993M 1.993M 1.993M 1.993M 1.993H 1.993H 1.7916 1.8920M 1.8920M 1.8777 1.8737 1.8145 1.8051 1.7916 1.7818 1.7916 1.7818 1.7607 1.7401 1.7546 1.7401 1.7527 1.6527 1.6405 1.6125 1.6084 1.5772 1.5441M 1.5373 1.5275 1.4736 1.4618M	2.945 10 2.891 12 2.850 9 2.810 19 2.732 80 2.648 10 2.542 14 2.512 13 2.430 4 2.415 4 2.341 17 2.247 25 2.214 13 2.188 6 2.177 13 2.140 4 2.046 4 2.041 13 1.993M 2 1.993M 1 1.993M 2 1.993M 1 1.993M 2 1.993M 1 1.993M 5 1.993M 1 1.993M 1 1.993M 1 1.993M 1 1.993M 1 1.993M 2 1.993M 1 1.993M 1 1.993M 1 1.993M 2 1.993M 1 1.993M 2 1.993M 1 1.993M 2 1.993M 3 1.9555 2 1.6405 5 1.6125 3 1.6405 5 1.6125 2 1.6084 3 1.5772 2 1.5441M 2 1.5441M 2 1.5441M 4	2.945 10 2 2 2.891 12 2 0 2.850 9 0 2 2.810 19 -2 2 2.648 10 -3 1 2.542 14 1 3 2.512 13 -1 1 2.430 4 1 1 2.415 4 1 3 2.341 17 2 2 2.247 25 0 2 2.214 13 3 1 2.188 6 4 0 2.177 13 -1 3 2.140 4 1 3 2.046 4 -2 2 2.041 13 0 0 1.993M 2 -3 1 1.993M 0 4 1.965 2 3 3 1.9361 4 0 4 1.9191 4 4 2 1.9036 11 1 1 1.8891 11 -2 0 1.8920M 12 -4 2 1.8920M 13 3 1.8777 12 4 0 1.8737 8 3 1 1.8145 3 2 4 1.8051 5 2 0 1.7916 4 0 4 1.7818 4 -2 4 1.7607 2 2 4 1.7401 6 3 3 1.8777 12 4 0 1.8737 8 3 1 1.8145 3 2 4 1.7607 2 2 4 1.7401 6 3 3 1.7105 1 5 1 1.6747 2 -2 4 1.7607 2 2 4 1.7401 6 3 3 1.7105 1 5 1 1.6747 2 -2 4 1.7607 2 2 4 1.7401 6 3 3 1.7105 1 5 1 1.6747 2 -2 4 1.7607 2 2 4 1.7507 2 2 4 1.7401 6 3 3 1.7105 1 5 1 1.6747 2 -2 4 1.7507 2 2 4 1.7507 2 2 4 1.7507 3 5 1 1.5441M 2 -4 0 1.5441M 2 -4 0 1.5441M 2 -5 4 1.55775 4 4 2 1.5441M 2 -4 0 1.5441M 2 -5 5 1.5373 3 1 5 1.5275 4 4 2 1.5441M 2 -4 0 1.5441M 2 -5 5	2.945

Sample The sample was made by treating NaHCO $_3$ and Al powder with HF solution. The precipitate was dried and heated to 450 °C for 10 minutes.

Color Colorless

Structure Tetragonal, P4/mnc (128), Z=2. The structure of $Na_5Al_3F_{14}$ was studied by Clausen [1936], and refined by Brosset [1938].

Lattice constants of this sample $a = 7.0142(8) \stackrel{\circ}{A}$

c = 10.400(3)

c/a = 1.4826

Volume o 511.6 Å³

Density (calculated) 2.998 g/cm³

Figure of merit $F_{30} = 61.2(0.014,35)$

Reference intensity
I/I = 1.15(5)

Additional pattern
1. PDF card 2-749 [Clausen, 1936] [Brosset, 1938]

References
Brosset, C., (1938). Z. Anorg. Allgem. Chem.
238, 201.
Clausen, H., (1936). Z. Kristallogr.
Kristallgeometrie Kristallphys.

Kristallchem. 95, 394.

CuKa ₁	a = 1.54059	8 Å;	tem	ρ.	25±1	°C	
Interna	ıl standard	Si,	a =	5	. 43088	B A	
d(A)	I		hkl			20	(°)
5.81	20	1	0	1		15.	
5.202	30	0	0	2		17.	.03
4.962	10	1	1	0		17.	
3.589	6	1	1	2		24.	
3.505	15	2	0	0		25.	. 39
3.107	3	1	0	3		28.	
3.004	18	2	1	1		29.	
2.909	100	2	0	2		30.	
2.601	7	0	0	4		34.	
2.481	8	2	2	0		36.	. 18
2.325	50	2	1	3		38.	
2.303	6	1	1	4		39.	
2.282	8	3	0	1		39.	
2.239	8	2	2	2		40.	
2.219	12	3	1	0		40.	62
2.170	20	3	1	1		41.	.58
2.089	2	2	0	4		43.	.27
2.040	2	3	1	2		44.	.38
2.002	25	2	1	4		45.	27
1.996	20	1	0	5		45.	39
1.946	11	3	2	0		46.	
1.940	7	3	0	3		46.	
1.7939	25	2	2	4		50.	
1.7537	23	4	0	0		52.	
1.7340M	5	2	1	5		52.	.75
1.7340M		0	0	6		52.	75
1.7020	2	4	1	0		53.	
1.6970	2	3	2	3		53.	
1.6875	6	3	1	4		54.	32
1.6786	6	4	1	1		54.	63
1.6615	3	4	0	2		55.	
1.6538	3	3	3	0		55.	52
1.6167	6	4	1	2		56.	91
1.5684	3	4	2	0		58.	
1.5538M	25	3	0	5		59.	44
1.5538M		2	0	6		59.	44
1.5013	19	4	2	2		61.	
1.4532M	7	4	0	4		64.	
1.4532M		1	0	7		64.	02
1.4284	1	4	2	3		65.	27
1.4208M	1	3	2	5		65.	66
1.4208M		2	2	6		65.	
1.4023	2	4	3	0		66.	
1.3945	4	3	3	4		67.	06
L							

CAS registry 1330-43-4	no
Sample The sample at 500 °C f	

is made by heating Na₂B₄O₇·10H₂O 72 hours.

Color Colorless

Structure

Triclinic, $P\bar{1}$ (2), Z = 4. The structure was refined by Krogh-Moe [1974].

Lattice constants of this sample

$$a = 8.646(4) \stackrel{\circ}{A}$$

 $b = 10.506(4)$

c = 6.572(2) $\alpha = 94.95(2)^{\circ}$

 $\beta = 90.93(4)$

y = 93.18(3)

a/b = 0.8229

c/b = 0.6255

Volume 593.7 Å³

Density

(calculated) 2.252 g/cm³

Figure of merit $F_{30} = 44.4 (0.014,49)$

Additional patterns

 PDF card 9-14 [Dasgupta and Banerjee, 1955]
 PDF card 27-656 [Smith et al., Annual Report to the Joint Committee on Powder Diffraction Standards, (1974)]

References

Dasgupta, D. R. and Banerjee, B. K. (1955). J. Chem. Phys. 23, 2189.

Krogh-Moe, J. (1974). Acta Crystallogr. B30, 578.

$CuK\alpha_1 \lambda = 1$	1.540598	A; temp	. 25±	1 °C
Internal st	andard S	i, a = 5	5.430	88 Å
d(A)	Ι	hkl		2Θ(°)
10.46	7	0 1	0	8.45
8.64	5	1 0	0	10.23
6.55	20	0 0	1	13.51
6.49	35	1 1	0	13.63
5.78	10	0 -1	1	15.32
5.35	25	0 1	1	16.57
5.23	50	0 2	0	16.93
5.17	17	1 0	1	17.13
4.83	4	1 -1	1	18.34
4.77	4	-1 -1	1	18.58

d(A)	I	hkl	2Θ(°)
4.64 4.360 4.321 4.072 3.926	8 30 20 25 100	-1 1 1 1 2 0 2 0 0 -2 1 0 0 2 1	19.12 20.35 20.54 21.81 22.63
3.879 3.779 3.647 3.484M 3.484M	12 2 6 19	1 -2 1 -1 -2 1 -1 2 1 0 3 0 2 -1 1	22.91 23.52 24.39 25.55 25.55
3.431+ 3.431+ 3.297 3.235 3.205	35 30 16 10	-2 -1 1 -2 1 1 -1 3 0 2 2 0 0 -1 2	25.95 25.95 27.02 27.55 27.81
3.086M 3.086M 3.035M 3.035M 2.998	16 10 8	2 -2 1 -1 0 2 1 -3 1 1 0 2 1 -1 2	28.91 28.91 29.41 29.41 29.78
2.972 2.859 2.841 2.815 2.790	8 11 17 35 20	0 3 1 -1 3 1 1 1 2 -3 1 0 -2 3 0	30.04 31.26 31.46 31.76 32.05
2.753 2.670 2.580M 2.580M 2.541	16 45 16	1 -2 2 0 2 2 2 0 2 -3 2 0 -1 4 0	32.50 33.54 34.74 34.74 35.29
2.513 2.459M 2.459M 2.412 2.374	15 50 8 6	-2 3 1 1 4 0 3 2 0 1 -3 2 -1 -4 1	35.70 36.51 36.51 37.25 37.87
2.287 2.240M 2.240M 2.176 2.160M	8 6 13 11	0 3 2 -1 3 2 1 4 1 0 -1 3 3 3 0	39.37 40.22 40.22 41.47 41.79
2.160M 2.134 2.121M 2.121M 2.087M	16 20 6	4 0 0 0 -4 2 -2 -4 1 -2 4 1 4 1 0	41.79 42.32 42.60 42.60 43.31
2.087M 2.052 2.040M 2.040M 2.034M	30 16 16	1 -4 2 3 -2 2 0 -5 1 4 0 1 -4 1 1	43.31 44.10 44.37 44.37 44.50
2.034M 2.022 1.936+ 1.936+ 1.923	25 30 25	-4 2 0 1 -2 3 -4 2 1 -1 4 2 -1 2 3	44.50 44.79 46.90 46.90 47.24

Sodium Borate, $Na_2B_4O_7$ (continued)

d(Å)	I	hkl	,	2Θ(°)
1.882+	10	- 4 3	0	48.33
1.882+		3 4	0	48.33
1.877	12	-3 4	1	48.45
1.870M	10	1 5	1	48.66
1.870M		-2 -2	3	48.66
1.865	10	2 1	3	48.80
1.837M	4	- 3 3	2	49.59
1.837M		0 -5	2	49.59
1.821M	8	-4 0	2	50.05
1.821M		-2 4	2	50.05
1.807	13	- 2 2	3	50.46
1.784	4	4 0	2	51.15
1.746	7	3 3	2	52.36
1.724	6	1 -4	3	53.09

Synonym 1. Tincal	CuKα ₁ λ	= 1.540598	8 A;	tem	p. 25±1	°C
CAS registry no.	Internal	standard	Si,	a =	5.4308	8 Å
1303-96-4	d(A)	I		hkl		2Θ(°)
Sample The sample from Fisher Scientific Co., Fairlawn, NJ was recrystallized from aqueous solution. It was somewhat unstable in dry air, losing H ₂ O to become the 5-hydrate. Because of this instability it was impossible to obtain	7.78 7.17 5.97 5.84 5.69	6 11 16 40 50	0 -1 1 2 0	1 1 0 0	1 1 0 2	11.36 12.34 14.83 15.15 15.56
consistent results with the intensity measure- ments.	5.33 5.20 4.860	7 20 80	0 -2 1	2 1 2	0 1 0	16.61 17.04 18.24
Color Colorless	3.936M 3.936M	45	-1 2		2 0	22.57
Structure Monoclinic, A2/a (15), Z = 4. The structure of borax was studied by Morimoto [1956], and refined by Levy and Lisensky [1978] using neutron diffraction.	3.889 3.596 3.577M 3.577M 3.498M	1 7 8	0 2 0 -2 -2	2 0 1 2 1	2 2 3 2 3	22.85 24.74 24.87 24.87 25.44
Lattice constants of this sample a = 12.219(3) Å b = 10.665(3) c = 11.884(2) β = 106.64(2)°	3.498M 3.391 3.334 3.187M 3.187M	2 3 8	1 0 -1 1 1	3 3	2 1 1 1 3	25.44 26.26 26.72 27.97 27.97
a/b = 1.1457 c/b = 1.1143 Volume	3.075 2.980 2.929 2.848 2.833	8 40 10 65 60	-3 2 4 0 2	2 2 0 0 3	2	29.01 29.96 30.50 31.39 31.55
1483.8 A ³ Density (calculated) 1.709 g/cm ³ Figure of merit F ₃₀ = 44.2(0.014,48)	2.740 2.676 2.665 2.644M 2.644M	1 4 9 5	2 -3	1 3 4	3 1 0 3 3	32.66 33.46 33.60 33.88 33.88
Additional patterns 1. PDF card 12-258 [Cipriani, 1958] 2. PDF card 24-1055 [Thomas and Soustelle, 1970] 3. Minder, W. [1935]	2.576 2.565M 2.565M 2.520 2.459	100 95 2 11	4 -2 4 3 3	1 3 2 2 3	1 3 0 2 1	34.80 34.95 34.95 35.60 36.51
References Cipriani, C. (1958). Atti Soc. Toscana Sci. Natur. Pisa Mem. Processi Verb. Ser. A 65, 284. Levy, H. A. and Lisensky, G. C. (1978). Acta	2.387 2.345 2.341 2.335 2.313	4 30 25 15 5	-3 4 3 -2 2	1	3 2 3 2 4	37.66 38.36 38.43 38.53 38.91
Crystallogr. <u>B34</u> , 3502. Minder, W. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. <u>92</u> , 301. Morimoto, N. (1956). Mineral J. Japan <u>2</u> , 1. Thomas, G. and Soustelle, M. (1970). Bull. Soc. Chim. Fr. <u>1970</u> , 4202.	2.258 2.218 2.201M 2.201M 2.174	1 9 8 5	-5 2 3 -4 -3	1 3 4 2 4	3 3 0 4 2	39.90 40.65 40.97 40.97 41.51
	2.162 2.146 2.122 2.098 2.081	6 8 2 4 10	-4 4 2 0 -1	3 2 2 5 5	3 2 4 1	41.74 42.07 42.56 43.09 43.46

Sodium Borate Hydroxide Hydrate (Borax), $Na_2B_4O_5(OH)_2 \cdot 8H_2O$ - (continued)

d(Å)	I	hkl	2Θ(°)
2.076 2.044 2.033 2.015 1.989	7 7 16 8 2	-4 1 5 1 5 1 -6 0 2 4 1 3 3 3 3	43.57 44.27 44.52 44.96 45.58
1.983M 1.983M 1.969M 1.969M 1.950M	3 5 9	-1 4 4 -4 4 2 -1 3 5 -2 3 5 3 4 2	45.71 45.71 46.05 46.05 46.53
1.950M 1.913M 1.913M 1.898 1.855M	12 11 9	6 0 0 -3 3 5 2 1 5 0 0 6 5 3 1	46.53 47.50 47.50 47.89 49.08
1.855M 1.833 1.790 1.777M 1.777M	12 4 5	-2 2 6 6 2 0 -4 4 4 4 3 3 0 6 0	49.08 49.71 50.98 51.39 51.39
1.758M 1.758M 1.748M 1.748M 1.731	10 3 2	-6 3 1 1 6 0 2 4 4 -4 5 1 -6 3 3	51.98 51.98 52.30 52.30 52.84
1.705M 1.705M 1.701M 1.701M 1.6613	8 11 2	2 5 3 2 3 5 -7 1 3 2 6 0 -3 1 7	53.73 53.73 53.84 53.84 55.25
1.6585+ 1.6585+ 1.6159M 1.6159M 1.5952	2 2 1	-7 2 2 1 6 2 -4 1 7 -6 4 2 7 2 0	55.35 55.35 56.94 56.94 57.75
1.5841M 1.5841M 1.5740M 1.5740M 1.5457+	1 2 2	-1 5 5 -2 5 5 6 4 0 7 1 1 0 4 6	58.19 58.19 58.60 58.60 59.78
1.5457+ 1.5313M 1.5313M 1.5197M 1.5197M	2	-5 1 7 -2 3 7 5 2 4 4 6 0 -3 3 7	59.78 60.40 60.40 60.91 60.91

d(Å)	I	hk	Q.	2Θ(°)
1.5177M	3	-1 3	-	61.00
1.5177M		-2 6	4	61.00
1.5083	3	0 6	4	61.42
1.4853	2	-4 3	7	62.48
1.4538	1	-4 0	8	63.99
1.4303M	5	6 3	3	65.17
1.4303M		- 5 3	7	65.17
1.4233	4	0 0	8	65.53
1.4153	3	2 4	6	65.95
1.3608M	2	- 5 2	8	68.95
				•
1.3608M		- 6 3	7	68.95

Sodium Silicon Fluoride (Malladrite), ${\rm Na_2SiF_6}$

Sample The sample was from Fisher Scientific Co., Fairlawn, NJ.
Color Colorless
Structure Hexagonal, P321 (150), Z = 3, isostructural with Na ₂ GeF ₆ and other hexafluorides. The structure is similar to that of $K_2S_2O_6$. The structure of Na ₂ SiF ₆ was determined by Zalkin et al. [1964].
Lattice constants of this sample
$a = 8.8659(7) \stackrel{\circ}{A}$ c = 5.0433(5)
c/a = 0.5688
Volume o 343.3 A ³
Density (calculated) 2.729 g/cm ³
Figure of merit $F_{30} = 76.6(0.012,34)$
Reference intensity I/I corundum = 0.87(2)
Additional patterns 1. PDF card 8-36 [African Explosives and Chem. Ind., Transvaal, South Africa] 2. PDF card 19-1193 [U.S. Bureau of Mines, Albany, OR] 3. PDF card 25-1166 [Royal Ontario Museum,
Ontario, Canada], pattern is actually sylvite (KCl) 4. Cox [1954] 5. Cipriani [1955]
References Cipriani, C. (1955). Rend. Soc. Mineral. Ital. 10, 253. Cox, B. (1954). J. Chem. Soc. 1954, 3251. Zalkin, A., Forrester, J. D., and Templeton, D. H. (1964). Acta Crystallogr. 17, 1408.

$CuK\alpha_1 \lambda =$	1.540598	8 Å;	temp). I	25±1 °C
	standard	Sí,	a =	5.	43088 Å
d(Å)	I		hkl		20(°)
5.041	13	0	0	1	17.58
4.429	100	1	1	0	20.03
4.213	95	1	0	1	21.07
3.331 3.056	90 50	1 2	1	1	26.74 29.20
3.030	50		J	•	
2.902	9	2	1	0	30.79
2.558	5	3	0	0	35.05
2.521 2.516	7 15	0 2	0 1	2	35.58 35.66
2.316	15 1	1	0	2	37.54
				_	
2.281	90	3	0	1	39.47
2.216	6	2	2	0	40.68
2.191	4	1	1 1	2	41.16 42.42
2.129 2.107	3 4	3 2	0	2	42.42 42.88
2.10/			J	_	
2.030	9	2	2	1	44.61
1.9626	6	3	1	1	46.22
1.9043	10	2	1	2	47.72
1.7962	55 /	3	0 2	2	50.79
1.7616	4	3	2	U	51.86
1.6806	2	0	0	3	54.56
1.6629	20	3	2	1	55.19
1.6419	4	1	0	3	55.96
1.6269	9	3	1	2	56.52
1.5904	20	4	1	1	57.94
1.5718	4	1	1	3	58.69
1.5404	3	2	0	3	60.01
1.5268	3	4	0	2	60.60
1.4776	11	3	3	0	62.84
1.4695	5	5	0	1	63.23
1.4548	8	2	1	3	63.94
1.4514	8	4		0	64.11
1.4049	3	3	0	3	66.50
1.3951M	8	4	1	2	67.03
1.3951M		4	2	1	67.03
1.3391	1	2	2	3	70.23
1.3302	3	5	1	1	70.77
1.3194	2	3	1	3	71.44
1.2751	1	3	3	2	74.33
1.2643	2	4	0	3	75.07
1.2609	2	0	0	4	75.31
1.2293	4	5	2	0	77.60
1.2160	3	3	2	3	78.61
1.2099	2	5	1	2	79.09
1.1869	1	4	1	3	80.93
1 1566	1	2	1	4	83.52
1.1566 1.1411	1 2	6	0	2	84.92
1.1312	3	3	0	4	85.84

CAS registry no. 12034-36-5 Sample The sample was prepared by dry heating Na_2CO_3 + TiO_2 (anatase) at 1250 °C. Since Na evaporated, NaOH plus moisture was added to make a paste. The sample was then heated for 45 minutes at 1000 °C and then reheated for 17 hours at 950 °C after correcting with TiO2. Color Colorless Structure Monoclinic, $P2_1/m$ (11), Z = 2. The structure was determined by Andersson and Wadsley [1961]. Lattice constants of this sample a = 9.1279(7) Ab = 3.8032(5)c = 8.5621(7) $\beta = 101.60(1)^{\circ}$ a/b = 2.4001c/b = 2.2513Volume 291.17 Å³ Density (calculated) 3.441 g/cm³ Figure of merit $F_{30} = 115.3(0.008,32)$ Additional pattern 1. PDF card 14-85 [Andersson and Wadsley, 1961]

Andersson, S. and Wadsley, A. D. (1961).

Acta Crystallogr. 14, 1245.

Reference

CuKα ₁ λ	= 1.540598	3 Å; t	emp	25±1 °C
	standard	W, a	= 3.	16524 A
d(Å)	I	h	ıkl	2Θ(°)
8.95 8.40 6.84 5.587 4.469	7 100 4 30 7	1 0 -1 1 2	0 0 0 1 0 1 0 1 0 0	10.52 12.93 15.85
4.189 4.130 3.652 3.535 3.464	2 5 2 1 35	0 -1 2 1 0	0 2 0 2 0 1 0 2 1 1	21.50 24.35 25.17
3.422 3.142 3.005 2.982 2.897	5 18 7 20 6	-2 1 -3 3 2	0 2 1 1 0 1 0 0 1 0	28.38 29.71 29.94
2.856 2.817 2.799M 2.799M 2.791	7 8 12 7	-2 0 -1 0 2	1 1 1 2 1 2 0 3 0 2	31.74 31.95 31.95
2.699 2.645 2.635 2.618 2.588	5 8 9 16 7	-3 3 2 -2 1	0 2 0 1 1 1 0 3 1 2	33.86 34.00 34.22
2.543 2.527 2.358 2.346 2.282	6 6 3 4 1	-2 1 -3 3 -3	1 2 0 3 1 1 1 0 0 3	35.49 38.13 38.33
2.274 2.251M 2.251M 2.236 2.172	1L 1 2 2	-1 0 2 4 3	1 3 1 3 1 2 0 0 1 1	40.02 40.02 40.31
2.158 2.1050 2.0967 2.0643 2.0598	1 3 4 35 40	-2 1 0 -2 4	1 3 1 3 0 4 0 4 0 1	42.93 43.11 43.82
1.9558M 1.9558M 1.9271 1.9221 1.9009	6 2 1 20	-3 1 4 3 0	1 3 0 4 1 0 1 2 2 0	46.39 47.12 47.25
1.8607M 1.8607M 1.8547 1.8261M 1.8261M	2 3 2	3 1 0 4 -5	0 3 2 0 2 1 0 2 0 1	48.91 49.08 49.90

Sodium Titanium Oxide, $Na_2Ti_3O_7$ - (continued)

1.8149 1.8105 1.7998 1.7670 1.7333	10 7 2 1	-2 4 1 2 -4	1 1 2	4	50.23 50.36
1.7998 1.7670 1.7333	2 1 1	1 2			30.30
1.7670 1.7333	1	2	7		
1.7333	1			1	50.68
			0	4	51.69
1 7279		-4	1	3	52.77
	1L	-1	2	2	52.95
1.7120	1	-1	0	5	53.48
1.6815	1	5	0	1	54.53
1.6716	1	3	1	3	54.88
1.6663	3	- 5	0	3	55.07
1.6459+	7	4	1	2	55.81
1.6459+		- 5	1	1	55.81
1.6112	2	- 5	1	2	57.12
1.6071M	3	- 3	2	1	57.28
1.6071M		- 3	0	5	57.28
1.6030M	5	3	2	0	57.44
1.6030M		2	1	4	57.44
1.5964	2	4	0	3	57.70
1.5797	1	-1	2	3	58.37
1.5612	5	-1	1	5	59.13
1.5413	6	-2	1	5	59.97
1.5378M	6	5	1	1	60.12
1.5378M		5	0	2	60.12
1.5195M	4	- 5	0	4	60.92
1.5195M		1	2	3	60.92
1.5024	2	-6	0	2	61.69
1.4934	1	-4	0	5	62.10
1.4902	1	6	0	0	62.25
1.4759	4	2	0	5	62.92
1.4720	6	4	1	3	63.11
1.4410	6	-6	0	3	64.63
1.4257M	2	-1	0	6	65.41
1.4257M		5	1	2	65.41
1.4117M	5	-6	1	1	66.14
1.4117M		- 5	1	4	66.14
1.3980M	14	-2	2	4	66.87
1.3980M	- '	ō	0	6	66.87
1.3969M	14	-6	1	2	66.93
1.3969M		4	2	1	66.93
1.3874	1	6	1	0	67.45
1.3759M	6	-3	0	6	68.09
1.3759M		2	1	5	68.09
1.3631	2	1	2	4	68.82
1.3507	1	3	0	5	69.54
1.3473	1L	- 6	1	3	69.74
1.3347	1	-1	1	6	70.50

CAS registry no. 12206-20-1

Sample

The sample was made by heating Cr_2O_3 with $SrCrO_4$ and $Sr(OH)_2$ under N_2 at about 1000 °C for about 1/2 hour.

Color Black

Structure

Orthorhombic, P2₁nb (33), Z = 8. The structure of Sr₂CrO₄ has been studied by Wilhelmi [1967].

Lattice constants of this sample

a = 10.007(2) Å b = 14.194(3) c = 5.809(1)

a/b = 0.7050c/b = 0.4093

Volume 825.1 A³

Density (calculated) 4.689 g/cm³

Figure of merit $F_{30} = 66.2(0.012,38)$

Polymorphism

Kafalas and Longo [1972] report that $\rm Sr_2CrO_4$ transforms to a $\rm K_2NiF_4$ structure at 65 kbars and 1000 °C.

Additional pattern

1. PDF card 19-1206 [Wilhelmi, 1967]

References

Kafalas, J. A. and Longo, J. M. (1972).
J. Solid State Chem. 4, 55.
Wilhelmi, K.-A., (1967). Ark. Kemi 26, 157.

CuΚα ₁ λ :	= 1.540598	À;	temp). 2	25±1 °C
	standard	Si,	a =	5.4	43088 Å
d(A)	I		hkl		2Θ(°)
5.024 5.007 3.663M 3.663M 3.448	3 2 4 3	1 2 0 2 1	0 0 3 1 3	1 0 1 1	17.64 17.70 24.28 24.28 25.82
3.343M 3.343M 3.029 3.021 2.901	17 19 16 90	1 2 0 3 1	4 2 4 2 4	0 1 1 0 1	26.64 26.64 29.47 29.54 30.80
2.892M 2.892M 2.848 2.738 2.680	100 8 2 1	2 3 0 1 3	4 0 1 1 2	0 1 2 2 1	30.89 30.89 31.39 32.68 33.41
2.592 2.550 2.512 2.472M 2.472M	5 2 3 4	2 0 2 2 1	4 5 0 1 5	1 1 2 2 1	34.58 35.16 35.72 36.31 36.31
2.430 2.403 2.368M 2.368M 2.360	20 2 5	3 1 2 0 4	4 3 2 6 2	0 2 2 0 0	36.96 37.39 37.97 37.97 38.10
2.303 2.273 2.267 2.247 2.243	7 1 1 1 1L	1 2 4 0 3	6 5 1 4 4	0 1 1 2	39.09 39.61 39.72 40.10 40.18
2.219 2.193M 2.193M 2.187 2.165	6 5 8 3	2 1 0 4 3	3 4 6 2 1	2 2 1 1 2	40.63 41.13 41.13 41.25 41.69
2.139 2.092 2.050 1.9878 1.9252	3 6 18 3 9	2 3 2 3 5	6 2 4 3 2	0 2 2 2 0	42.22 43.20 44.15 45.60 47.17
1.8916 1.8791 1.8636 1.8344 1.8038	4 3 9 1 2	5 4 3 0 1	0 1 4 6 6	1 2 2 2 2	48.06 48.40 48.83 49.66 50.56
1.7916M 1.7916M 1.7743 1.7641 1.7500	3 1 3 4	0 2 0 1 2	3 1 8 3 2	3 3 0 3 3	50.93 50.93 51.46 51.78 52.23

Strontium Chromium Oxide, Sr_2CrO_4 - (continued)

d(Å)	I	hkl		2θ(°)
1.7438	5	5 4	0	52.43
1.7340	3	3 5	2	52.75
1.7221	1	2 6	2	53.14
1.6996	3	0 4	3	53.90
1.6872	1	2 3	3	54.33
1.6744	11	3 0	3	54.78
1.6716	13	4 4	2	54.88
1.6632M	6	3 1	3	55.18
1.6632M		0 7	2	55.18
1.6486	7	4 6	1	55.71
1.6368	2	5 1	2	56.15
1.6087	7	2 4	3	57.22
1.6058	4	5 2		57.33
1.5789M	2	1. 5	2 3 3	58.40
1.5789M		3 3	3	58.40
1.5658	5	3 8	0	58.94
1.5636	2	6 2	1	59.03

CAS registry no. 7440-28-0

Sample

The sample was obtained from the Fisher Scientific Co., Silver Spring, MD.

Color

Gray metallic

Structure

Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with magnesium. The structure of thallium was studied by Sekito [1930].

Lattice constants of this sample

a = 3.4568(3) Ac = 5.5259(5)

c/a = 1.5986

Volume 57.185 A³

Density

(calculated) 11.869 g/cm³

Figure of merit $F_{22} = 76.9(0.012,24)$

Polymorphism

Hexagonal thallium transposes to a bodycentered cubic phase above 230 °C [Lipson and Stokes, 1941]. Becker and Ebert [1923] had reported a tetragonal phase which later was shown to be hexagonal.

Additional patterns

- 1. PDF 1-1084 [Hanawalt et al., 1938]
- 2. Barrett [1958]
- 3. Sekito [1930]
- 4. Suganuma [1960]

References

Barrett, C. S. (1958). Phys. Rev. 110, 1071.

Becker, K. and Ebert, F. (1923). Z. Phys. 16,

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457. Lipson, H. and Stokes, A. R. (1941). Nature 148,

Sekito, S. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 74, 189.

Suganuma, R. (1960). J. Phys. Soc. Japan. 15,

CuKα ₁ λ	= 1.54059	8 A;	tem	p. 2	5±1 °C
	standard	W, a	=	3.16	524 Å
d(A)	I		hkl		2Θ(°)
2.991	20	1	0	0	29.85
2.760	50	0	0	2	32.41
2.631	100	1	0	1	34.05
2.030	20	1	0	2	44.59
1.7285	18	1	1	0	52.93
1.5687	35	1	0	3	58.82
1.4965	3	2	0	0	61.96
1.4651	20	1	1	2	63.44
1.4447	14	2	0	1	64.44
1.3820	8	0	0	4	67.75
1.3159	3	2	0	2	71.66
1.2544	7	1	0	4	75.77
1.1617	9	2	0	3	83.07
1.1084	10	2	1	1	88.05
1.0792	11	1	1	4	91.09
1.0473	2	2	1	2	94.70
1.0368	16	1	0	5	95.97
1.0151	3	2	0	4	98.72
. 9980	3	3	0	0	101.04
.9640	6	2	1	3	106.08
. 9386	3	3	0	2	110.30
.9210	3 3	0	0	6	113.52

CAS registry no. 7789-27-7
Sample The sample was obtained from the City Chemical Co., New York, NY.
Color Colorless
Structure Orthorhombic, Z = 4. Pca* is consistent with the absences and has been used without any verifying data. Ketelaar [1935] determined that TIF belonged to the space group Fmmm (69) However, data reported here, as well as data from another researcher, Harshaw (priv. comm.) have a number of weak extra lines which do not fit that space group. These extra lines were found to persist after the sample had been refluxed.
Lattice constants of this sample
a = 5.4910(4) Å $b = 6.0974(3)$ $c = 5.1855(4)$
a/b = 0.9006 c/b = 0.8504
Volume o 173.61 A ³
Density (calculated) 8.546 g/cm ³
Figures of merit $F_{30} = 44.6(0.010,70)$ $M_{20} = 71.0$
Reference intensity I/I = 3.2(3)
Additional pattern 1. PDF 3-0483 [Ketelaar, 1935]
Reference Ketelaar, J. A. A. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. <u>92</u> , 30.

CuKα ₁ λ =	= 1.540598	8 A; 1	temp	. 25±1	°C
Internal	standard	W, a	= 3	. 16524	o A
d(Å)	I	ì	nkl		2θ(°)
6.095 3.205 3.047 2.748 2.593	1 100 45 16 16	0 1 0 2 0	1 1 2 0 0	0 1 0 0 2	14.52 27.81 29.29 32.56 34.56
2.426 2.370 2.0400 1.9755 1.8857	1 2 13 11 11	2 1 2 0 2	0 2 2 2 0	1 1 0 2 2	37.02 37.93 44.37 45.90 48.22
1.7889 1.6604 1.6033 1.5916 1.5243	20 8 10 8 4	1 3 2 1 0	3 1 2 1 4	1 1 2 3 0	51.01 55.28 57.43 57.89 60.71
1.4134 1.3727 1.3327 1.3143 1.2965M	1L 1 3 5	1 4 2 0 4	4 0 4 4 1	1 0 0 2 1	66.05 68.27 70.62 71.76 72.90
1.2965M 1.2807 1.2517 1.2307 1.2194	4 1 3 1L	0 1 4 3 0	0 3 2 1 5	4 3 0 3 0	72.90 73.95 75.96 77.50 78.35
1.2129 1.1930 1.1897 1.1854 1.1717	1 1 1 3 1	4 0 4 2 3	0 2 1 4 4	2 4 2 2 0	78.85 80.43 80.70 81.06 82.21
1.1601 1.1273 1.1111 1.1037 1.0940	4 1 1L 1L 2	1 4 4 0 2	5 2 3 5 2	1 2 1 2 4	83.21 86.21 87.78 88.52 89.52
1.0690 1.0583 1.0201 1.0164 .9959	2 2 1 1	3 5 4 0 3	3 1 4 6 5	3 1 0 0 1	92.20 93.42 98.07 98.56 101.33
.9876 .9805 .9719 .9530 .9493	1L 1 1L 1	0 1 1 2 4	4 5 4 6 4	3 4 0	102.52 103.55 104.85 107.85 108.47
.9461 .9291 .9111 .9004 .8945	1 1 1 1	0 2 1 4 2	6 4 3 2 6	4 5 4	109.01 112.00 115.45 117.64 118.89
.8751 .8486	1 1	3 1	5 7		123.34 130.38

Thallium Hydrogen Phthalate, C₈H₅O₄Tl

Synonyms

1. Thallous acid phthalate

2. Thallium hydrogen-o-phthalate

CAS registry no. 29050-41-7

Sample

The sample was obtained as fragments of a single crystal, originally from Quartz Products, Plainfield, NJ.

Color

Colorless

Structure

Orthorhombic, $Pca2_1$ (29), Z = 4, by analogy with $C_8H_5O_4Rb$. The structure of $C_8H_5O_4Rb$ was refined by Smith [1975].

Lattice constants of this sample

a = 10.050(2) A

b = 12.882(2)

c = 6.622(1)

a/b = 0.7802

c/b = 0.5140

Volume 857.2 A³

Density

(calculated) 2.863 g/cm³

Figure of merit

 $F_{30} = 54.7(0.014,40)$

Reference

Smith, R. A. (1975). Acta Crystallogr. <u>B31</u>, 2347.

CuK α_1 λ = 1.540598 $\overset{\circ}{A}$; temp. 25±1 °C Internal standard Si, a = 5.43088 $\overset{\circ}{A}$

Internal	standard	Si,	a =	5.	43088 A
d(Å)	I		hkl		2Θ(°)
12.91 7.91 6.44 5.43 5.084	100 1L 11 3 4	0 1 0 1 1	1 1 2 2 1	0 0 0 0	6.84 11.18 13.73 16.32 17.43
5.029 4.684 4.296 4.197 4.005	2 1 3 4 12	2 2 0 1 2	0 1 3 2 0	0 0 0 1	17.62 18.93 20.66 21.15 22.18
3.952 3.824 3.397 3.311 3.220	9 25 25 2 10	1 2 2 0 0	3 1 2 0 4	0 1 1 2 0	22.48 23.24 26.21 26.91 27.68
3.066 2.972 2.944 2.930 2.825	5 4 8 7 3	1 3 0 2 1	4 2 2 3 2	0 0 2 1 2	29.10 30.04 30.34 30.48 31.65
2.783 2.708M 2.708M 2.643 2.624	6 2 3 2	1 3 2 3 0	4 2 4 3 3	1 1 0 0 2	32.14 33.05 33.05 33.89 34.14
2.577 2.538 2.510M 2.510M 2.496	1L 2 4	0 1 4 2 1	5 3 0 4 5	0 2 0 1 0	34.78 35.34 35.74 35.74 35.95
2.466 2.336 2.323M 2.323M 2.250	3 7 4	4 1 2 3 1	1 5 3 4 4	0 1 2 0 2	36.41 38.51 38.73 38.73 40.05
2.210 2.169 2.147 2.099 2.063	3 1L 1L 1L 3	3 4 0 1 3	2 3 6 6 3	2 0 0 0 2	40.79 41.61 42.05 43.05 43.84
2.060 2.042 2.021 2.001 1.997	2 3 2 6 6	4 3 2 1 2	3 5 0 6 1	1 0 3 1 3	43.91 44.32 44.80 45.28 45.38
1.978 1.952 1.927M 1.927M 1.911	3 1L 2	4 3 2 1 4	1 5 2 3 2	2 1 3 3 2	45.85 46.48 47.12 47.12 47.54

Thallium Hydrogen Phthalate, $C_8H_5O_4T1$ - (continued)

d(A)	I	hkl		2Θ(°)
1.901M	3	5 1	1	47.80
1.901M		3 4	2	47.80
1.840	1L	0 7	0	49.49
1.829	1	2 3	3	49.82
1.809	2	1 7	0	50.40
1.792	1	1 4	3	50.93
1.773	1L	1 6	2	51.49
1.755	1	5 3	1	52.07
1.746	1	1 7	1	52.35
1.7392	2	3 5	2	52.58
1.6996	1L	4 4	2	53.90
1.6953	1L	2 6	2	54.05
1.6713	1L	2 7	1	54.89
1.6522M	2	1 5	3	55.58
1.6522M		5 4	1	55.58
1.6416	1	0 1	4	55.97
1.6198M	1L	6 2	0	56.79
1.6198M		1 1	4	56.79
1.6094M	1	0 8	0	57.19
1.6094M		0 7	2	57.19
1.5861	1	3 6	2	58.11
1.5455M	1	1 8	1	59.79
1.5455M		0 3	4	59.79
1.5415	1	5 5	1	59.96
1.5209	1L	1 6	3	60.86
				(0.00
1.4937	1L	2 8	1	62.09
1.4842M	1L	6 1	2	62.53
1.4842M		4 7	0	62.53

The experimental data reported here are the same as those reported earlier by Swanson and Fuyat [1953]. This pattern has not been remeasured. The space group has been changed and the corresponding indices were changed when necessary. Also other additional information has been added.

CAS registry no. 1314-12-1

Sample

The sample of thallium oxide from Johnson Matthey Co., Ltd., London, England, was annealed at 370 °C in a sealed tube for 2 hours to prevent volatilization of noxious fumes.

Major impurities

0.001 to 0.01% each: Ca, Mg, Li, and Na less than 0.001% each: Al, Cu, Pb, and Si.

Color Black

Structure

Cubic, Ia3 (206), Z = 16, isostructural with Mn_2O_3 [Pauling and Shappell, 1930]. The space group used earlier was $I2_13$.

Lattice constant of this sample a = 10.5434(7) A

Volume 1172.0 Å³

Density

(calculated) 10.354 g/cm³

Figure of merit $F_{30} = 52.7(0.018,31)$

Polymorphism
Prewitt et al. [1969] report the existence of a hexagonal modification.

Additional patterns

1. PDF card 5-584 [Swanson and Fuyat, 1953]

2. Hanawalt et al. [1938]

Kon'kova and Savel'ev [1960], natural mineral

References

Hanawalt, J. D., Rinn, H. W., and Frevel,
 L. K. (1938). Ind. Eng. Chem. Anal.
 Ed. <u>10</u>, 457.

Kon'kova, E. A. and Savel'ev, V. F. (1960). Zap. Vses. Mineral. Obshchest. 89, 316.

Pauling, L. and Shappell, M. D. (1930).

Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 75, 128. Prewitt, C. T., Shannon, R. D., Rogers,

D. B., and Sleight, A. W. (1969). Inorg. Chem. 8, 1985.

Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. U.S. Circ. 539, 2, 28.

CuKα ₁	$\lambda = 1.540598$	A;	temp	25±1	°C
Intern	al standard	W, a	= 3	3.16524	o A
d(Å)	I		hkl		2Θ(°)
4.304	11	2	1	1	20.62
3.042	100	2	2	2	29.34
2.816	3	3	2	1	31.75
2.635	42	4	0	0	34.00
2.484 2.357 2.248 2.149 2.068 1.924	6 2 4 1 8 3	4 3 4 4 5	1 2 3 2 3 2	1 0 2 2 1	36.13 38.15 40.08 42.01 43.74 47.20
1.863 1.808 1.758 1.710 1.668	33 2 1 5	4 4 6 6 6	4 3 0 1 2	0 3 0 1	48.85 50.43 51.97 53.55 55.01
1.6280	4	5	4	1	56.48
1.5890	27	6	2	2	57.99
1.5540	6	6	3	1	59.43
1.5220	6	4	4	4	60.81
1.4910	3	5	4	3	62.21
1.4620	i	6	4	0	63.59
1.4340	3	6	3	3	64.98
1.4090	2	6	4	2	66.28
1.3390	3	6	5	1	70.24
1.3180	3	8	0	0	71.53
1.2980	4	7	4	1	72.80
1.2790	2	8	2	0	74.06
1.2597	2	6	5	3	75.40
1.2428	1	6	6	0	76.60
1.2261	3	8	3	1	77.84
1.2094	6	6	6	2	79.13
1.1789	4	8	4	0	81.60
1.1646	1	8	3	3	82.82
1.1371	2	9	2	1	85.29
1.1110	1	7	5	4	87.79
1.0874	1	9	3	2	90.21
1.0764	2	8	4	4	91.39
1.0649	1	9	4	1	92.66

Synonyms 1. 2,6,8-Trioxypurine 2. 8-Hydroxyxanthine
CAS registry no. 69-93-2
Sample The sample was NBS Standard Reference Material 913.
Color Colorless
Structure Monoclinic, $P2_1/n$ (14), $Z = 4$. The structure was determined by Ringertz [1966].
Lattice constants of this sample
a = 13.102(3) A b = 7.416(2) c = 6.225(1) β = 90.37(3)°
a/b = 1.7667 c/b = 0.8394
Volume 604.9 Å ³
Density (calculated) 1.846 g/cm ³
Figure of merit F ₃₀ = 36.3(0.012,68)
Reference intensity I/I corundum = 0.94(1)
Polymorphism Shirley and Sutor [1968] report a second phase with a monoclinic cell of similar size.
Additional patterns 1. PDF card 21-1959 [Shirley and Sutor, 1968] 2. PDF card 22-2000 [Swanson et al., 1970]
References Ringertz, H. (1966). Acta Crystallogr. <u>20</u> , 397.
Shirley, R. and Sutor, D. J. (1968). Science 159, 544.
Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1970). Nat. Bur. Std. U.S. Monogr. <u>25</u> , Sec. 8, 154.

	CuKα ₁ λ :	= 1.540598	о А;	tem	p 25	5±1 °C
		standard	Ag,	a =	4.0	08651 Å
	d(Å)	I		hkl		2Θ(°)
	6.54	45	2	0	0	13.53
	5.633	18	-1	0	1	15.72
	4.913	50	2	1	0	18.04
	4.769	7	0	1	1	18.59
	4.485	2	-1	1	1	19.78
	3.860	55	-2	1	1	23.02
	3.706	7	0	2	0	23.99
	3.587	4	- 3	0	1	24.80
	3.276	17	4	0	0	27.20
	3.185	50	0	2 ·	1	27.99
	3.098	100	-1	2	1	28.79
	2.994	4	4	1	0	29.82
	2.868M	25	0	1	2	31.16
	2.868M		-2	2	1	31.16
	2.801	11	1	1	2	31.93
	2.623	3	2	1	2	34.15
1	2.570	16	3	2	1	34.88
	2.456	3	4	2	0	36.56
	2.421	4	-5	0	1	37.11
	2.312	4	2	3	0	38.92
	2.280	5	4	2	1	39.50
	2.245	11	-2	2	2	40.14
	2.184	6	6	0	0	41.31
1	2.151M	2	4	1	2	41.96
	2.151M		3	3	0	41.96
	2.096M	2	-3	2	2	43.12
	2.096M		6	1	0	43.12
	2.032	3	3	3	1	44.56
1	2.027	3	-5	2	1	44.67
	1.997	1L	0	1	3	45.37
	1.989	1L	-6	1	1	45.56
	1.978	1L	-1	1	3	45.84
	1.9306M	1	-4	2	2	47.03
	1.9306M		5	1	2	47.03
	1.9149+	1	-2	1	3	47.44
	1.9149+		1	3	2	47.44
	1.8821M	2	-4	3	1	48.32
	1.8821M		6	2	0	48.32
	1.8788M	2	- 3	0	3	48.41
	1.8788M		4	3	1	48.41
	1.8697	1	3	0	3	48.66
	1.7988M	6	6	2	1	50.71
	1.7988M		5	3	0	50.71
	1.7955M	5	-7	0	1	50.81
	1.7955M		-1	2	3	50.81

CAS registry no. 13637-61-1

Sample

The sample was prepared by evaporation at room temperature of an aqueous solution.

Color Colorless

Structure

Hexagonal, P6/mmm (191), Z = 4, isostructural with Ni and other divalent metal perchlorate hexahydrates. The structure of this group of compounds was studied by West [1935].

Lattice constants of this sample

a = 15.629(4) Ac = 5.215(1)

ì

c/a = 0.3337

Volume 0 1103.1 Å³

Density (calculated) 2.242 g/cm³

Figure of merit $F_{30} = 32.3(0.012,77)$

Additional pattern
1. PDF card 6-197 [Dow Chemical Co.]

Reference

West, C. D. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. <u>91</u>, 480.

CuK $lpha_1$	$\lambda = 1.540598$	Ä;	tem	р.	25±1 °C
Intern	al standard	Ag,	a =	4.	.08651 Å
d(Å)	I		hkl		2Θ(°)
6.77	6	2	0	0	13.06
4.868	14	1	0	1	18.21
4.341	6	1	1	1	20.44
4.132	85	2	0	1	21.49
3.909	100	2	2	0	22.73
3.655	6	2	1	1	24.33
3.386	3	4	0	0	26.30
3.045	2	3	1	1	29.31
2.841	75	4	0	1	31.46
2.670	3	3	2	1	33.54
2.608	12	0	0	2	34.36
2.560M	3	1	0	2	35.03
2.560M	7.0	4	2	0	35.03
2.433M	10	2	0	2	36.91
2.433M		5	1	0	36.91
2.296	11	4	2	1	39.21
2.258M	6	3	0	2	39.90
2.258M		6	0	0	39.90
2.168M	4	2	2	2	41.62
2.168M		5	2	0	41.62
2.072	8	6	0	1	43.66
2.066M	18	4	0	2	43.79
2.066M		6	1	0	43.79
1.955M	12	4	1	2	46.42
1.955M		4	4	0	46.42
1.878M	6	5	0	2	48.42
1.878M		6	2	0	48.42
1.826	22	4	2	2	49.91
1.7657	9	6	2	1	51.73
1.7058M	5	6	0	2	53.69
1.7058M		6	3	0	53.69
1.6950	2	7	1	1	54.06
1.6838	4	2	0	3	54.45
1.6089	2	8	0	1	57.21
1.5462	5	4	0	3	59.76
1.5236M	4	6	2	2	60.74
1.5236M	_	7	3	0	60.74
1.4768M	7	7	1	2	62.88
1.4768M	17	8	2	0	62.88
1.4626	1L	5	0	3	63.56
1.4372	1	4	2	3	64.82
1.4193M	4	8	0	2	65.74
1.4193M		6	5	0	65.74

CAS registry no. 7779-90-0
Sample The sample was prepared by heating ${\rm ZnCO_3}$ and ${\rm P_2O_5}$ at 900 °C for several days with intermittent grindings.
Color Colorless
Structure Monoclinic, A2/a (15), $Z = 4$. The structure was determined by Calvo [1965].
Lattice constants of this sample
$a = 15.006(3) \text{ Å}$ $b = 5.635(1)$ $c = 8.183(1)$ $\beta = 104.99(2)^{\circ}$
a/b = 2.6629 c/b = 1.4521
Volume 668.5 A ³
Density 3.836 g/cm ³
Figure of merit $F_{30} = 37.4(0.016,51)$
Reference intensity I/I _{corundum} = 1.40(9)
Polymorphism Above 942 °C, α - $Zn_3(PO_4)_2$ transforms to β - $Zn_3(PO_4)_2$. A small percentage of Mn++ substituting for the Zn++ stabilizes a γ form [Calvo, 1965].
Additional patterns
1. PDF card 1-524 [New Jersey Zinc Co.] 2. PDF card 11-35 [Katnack and Hummel, 1958]
References Calvo, C. (1965). Can. J. Chem. <u>43</u> , 436. Katnack, F. L. and Hummel, F. A. (1958). J. Electrochem. Soc. <u>105</u> , 125.

CuK α_1	$\lambda = 1.54059$	8 Å;	temp	. 2	25±1 °C
	nal standard	Ag,	a =	4.0	8651 Å
d(Å)	I		hkl		2Θ(°)
7.25 4.583M 4.583M 4.193 3.947	3 35 30 35	2 0 -1 1 0	0 1 1 1 0	0 1 1 1 2	12.20 19.35 19.35 21.17 22.51
3.928	25	-2	0	2	22.62
3.607	90	-3	1	1	24.66
3.146	70	2	0	2	28.35
3.079	100	-4	1	1	28.98
2.815	13	0	2	0	31.76
2.764	9	1	2	0	32.36
2.657	9	4	1	1	33.70
2.627	20	2	2	0	34.10
2.448	40	-1	1	3	36.68
2.415	20	6	0	0	37.20
2.385	6	0	1	3	37.68
2.320	5	-1	2	2	38.78
2.294	35	0	2	2	39.24
2.287	16	-2	2	2	39.36
2.250	25	-4	1	3	40.04
2.225	18	4	2	0	40.51
2.216	16	1	2	2	40.68
2.125	12	2	1	3	42.50
2.086	12	-4	2	2	43.34
2.018	5	6	1	1	44.89
1.975 1.963M 1.963M 1.941 1.859	11 11 5 5	0 3 -4 -6 6	0 2 0 1 0	4 2 4 3 2	45.90 46.21 46.21 46.76 48.97
1.837 1.827M 1.827M 1.805 1.789	13 16 10 9	-8 -1 0 -6 7	0 3 3 2 1	2 1 1 2 1	49.59 49.87 49.87 50.52 51.00
1.785	12	-7	1	3	51.14
1.745	1	-3	3	1	52.39
1.6761	11	3	3	1	54.72
1.6727	9	-4	3	1	54.84
1.6552	7	-2	2	4	55.47
1.6175	2	0	2	4	56.88
1.5957	5	-9	1	1	57.73
1.5677	3	-3	1	5	58.86
1.5502	17	-8	0	4	59.59
1.5479	16	-4	1	5	59.69
1.5281 1.5229 1.5115M 1.5115M	1	6 0 -5 2 5	1 1 1 2 3	3 5 5 4 1	60.54 60.77 61.28 61.28 61.47
1.5072+		8	0	2	61.47
1.4980	6	1	3	3	61.89
1.4759	5	1	1	5	62.92

registry 779-90-0	no.

Sample The sample was prepared by heating ${\rm ZnCO_3}$ and ${\rm H_3PO_4}$ together at 1000 °C for several days, and cooling rapidly.

Color Colorless

Structure Monoclinic, $P2_1/a$ (14), Z=4. The structure of β - $Zn_3(P0_4)_2$ was determined by Stephens and Calvo [1967].

Lattice constants of this sample

a = 8.685(2) A b = 9.179(1) c = 8.265(1) $\beta = 112.80(1)^{\circ}$

a/b = 0.9462c/b = 0.9004

Volume 607.5 A³

Density (calculated) 4.221 g/cm³

Figure of merit $F_{30} = 88.4(0.009,36)$

Polymorphism $Zn_3(PO_4)_2$ has an inversion from α to β form at 942 °C. This is sluggish so that the β (high) form exists metastably at room temperature. [Stephens and Calvo, 1967] [Katnack and Hummel, 1958].

Additional pattern
1. PDF card 11-27 [Katnack and Hummel, 1958]

References
 Katnack, F. L. and Hummel, F. A. (1958). J.
 Electrochem. Soc. 105, 125.
 Stephens, J. S. and Calvo, C. (1967). Can.
 J. Chem. 45, 2303.

0	l standard				
d(A)	I		hkl		2Θ(°)
7.61	3	0	0	1	11.62
6.04	2	1	1	0	14.66
5.590	2	-1	1	1	15.84
4.296	5	-2	0	1	20.66
4.178	12	1	1	1	21.25

d(Å)	I	hkl	2Θ(°)
4.008 3.931 3.890 3.810 3.753	9 35 25 3 2	2 0 0 0 2 1 -2 1 1 0 0 2 -1 1 2	22.16 22.60 22.84 23.33 23.69
3.669 3.526 3.290 3.135 3.084	14 9 100 35 45	2 1 0 -2 0 2 -2 1 2 -2 2 1 2 0 1	24.24 25.24 27.08 28.45 28.93
3.064 3.018 2.931 2.927 2.866	55 30 10 7 80	-1 2 2 2 2 0 0 2 2 2 1 1 1 1 2	29.12 29.58 30.47 30.52 31.18
2.839 2.808 2.759 2.661 2.626	50 11 2 4 4	0 3 1 -1 3 1 -3 1 1 -2 0 3 -3 1 2	31.49 31.84 32.43 33.65 34.12
2.561+ 2.561+ 2.557 2.539 2.491	15 14 11 35	1 3 1 2 2 1 -2 1 3 0 0 3 -2 3 1	35.01 35.01 35.06 35.32 36.02
2.455 2.449M 2.449M 2.431 2.387	6 8 3 25	-1 3 2 0 1 3 -3 2 1 2 3 0 0 3 2	36.58 36.67 36.67 36.95 37.65
2.357 2.352 2.343 2.306 2.300	10 8 3 9	-1 2 3 -3 2 2 2 0 2 3 2 0 -2 2 3	38.15 38.23 38.38 39.02 39.13
2.296 2.269 2.206 2.197 2.182	11 3 6 14 5	0 4 0 2 1 2 1 4 0 0 4 1 -1 4 1	39.20 39.69 40.88 41.04 41.34
2.173 2.148M 2.148M 2.128 2.103	3 14 3 8	2 3 1 1 3 2 -4 0 2 1 1 3 -3 3 1	41.53 42.02 42.02 42.44 42.97
2.091M 2.091M 2.087 2.061 2.043M	18 16 1 3	-3 2 3 -4 1 2 2 2 2 1 4 1 -1 3 3	43.24 43.24 43.33 43.89 44.30
2.043M 2.028 2.024 2.007M 2.007M	9 10 11	-3 3 2 3 2 1 -2 4 1 -2 3 3 -2 1 4	44.30 44.64 44.74 45.14 45.14

Zinc Phosphate, β -Zn_3(PO_4)_2 - (continued)

0	т	h.1- 0		2Θ(°)
d(A)	I	hkl		20(*)
1.992M	8	- 4 0	3	45.51
1.992M		-1 1	4	45.51
1.976	1	1 2	3	45.89
1.965	2	0 4	2	46.15
1.954M	4	4 1	0	46.43
1.954M		0 3	3	46.43
1.945M	7	- 4 1	3	46.66
1.945M	·	-4 2	2	46.66
1.923	6	-2 4	2	47.22
1.9054M	14	-3 1	4	47.69
- 005/14		0 0	,	17.60
1.9054M	7	0 0	4	47.69
1.8766 1.8657	9	-2 2 0 1	4	48.47 48.77
1.8632M	25	-1 2	4	48.84
1.8632M	23	-3 3	3	48.84
1.005211		5 5	,	40.04
1.8597	20	2 3	2	48.94
1.8455	3	2 0	3	49.34
1.8344M	4	4 2	0	49.66
1.8344M	_	3 1	2	49.66
1.8268M	5	- 4 2	3	49.88
1.8268M		1 4	2	49.88
1.8098	5	2 1	3	50.38
1.7899	6	1 5	0	50.98
1.7750	9	4 0	1	51.44
1.7613+	3	-1 4	3	51.87
1.7613+		-4 3	1	51.87
1.7395	2	3 4	ō	52.57
1.7096	12	1 5	1	53.56
1.7034	10	0 4	3	53.77
1.6872	10	- 2 5	1	54.33
1.6772M	13	- 5 1	1	54.68
1.6772M	15	- 1 5	2	54.68
1.6699M	7	-4 3	3	54.94
1.6699M	·	2 5	0	54.94
1.6525M	8	-2 0	5	55.57
7 (505)			•	55 53
1.6525M 1.6427M	10	-5 1 -2 2	3	55.57
1.6427M	13	-3 3 -3 4	4 3	55.93 55.93
1.6280	5	-2 5	2	56.48
1.6240	6	- 5 2	2	56.63
1102.0	Ť	3 -	-	30103
1.6105	2	3 4	1	57.15
1.6023	9	1 2	4	57.47
1.5972M	6	3 3	2	57.67
1.5972M	3	-3 1 -1 1	5	57.67
1.5924	3	-1 1	5	57.86
1.5679M	12	1 5	2	58.85
1.5679M		-4 4	2	58.85
1.5557	2	-2 2	5	59.36
1.5502	4	- 3 5	1	59.59
1.5399	5	3 1	3	60.03

	d(Å)	I		hkl		20(°)
	1.5313M	7	-4	0	5	60.40 '
	1.5313M		-2	4	4	60.40
	1.5245+	6	-1	2	5	60.70
	1.5245+		-1	4	4	60.70
	1.5117+	7	5	2	0	61.27
	1.5117+		-2	5	3	61.27
	1.5083M	9	4	4	0	61.42
i	1.5083M		2	0	4	61.42
	1.5041M	10	-4	4	3	61.61
	1.5041M		0	1	5	61.61

Sample This sample was prepared by heating stoichiometric amounts of ZnCO ₃ and H ₃ PO ₄ with 3% of the ZnCO ₃ replaced by MnCO ₃ , at 900 °C for several days. This phase has useful luminescence properties, and is only stabilized by the addition of low percents of certain other bivalent cations [Calvo, 1965].
Color Colorless
Structure Monoclinic, $P2_1/n$ (14), $Z = 2$. The structure of γ - $Zn_3(P0_4)_2$ was determined by Calvo [1963].
Lattice constants of this sample a = 7.549(1) Å b = 8.499(1) c = 5.0491(8) β = 95.03(1)°
a/b = 0.8882 c/b = 0.5941
Volume o 322.7 Å ³
Density (calculated) 3.973 g/cm ³
Figure of merit F ₃₀ = 85.9 (0.009,37)
Reference intensity I/I corundum = 1.6(2)
Polymorphism Without the addition of other bivalent ions ${\rm Zn_3(PO_4)_2}$ exists in an α form below 942 °C and in a β form above. Both are monoclinic [Calvo, 1965].
Additional pattern 1. Hummel and Katnack [1958]
References Calvo, C. (1963). J. Phys. Chem. Solids. 24, 141. Calvo, C. (1965). Can. J. Chem. 43, 436. Hummel, F. A. and Katnack, F. L. (1958). J. Electrochem. Soc. 105, 528.

CuKα ₁ λ	= 1.540598	3 A;	temp	p .	25±1 °C
	standard	Si,	a =	5.	43088 A
d(Å)	I		hkl		2Θ(°)
5.626 4.363	6 80	1 -1	1 0	0 1	15.74 20.34
4.331 4.249	25 3	0	1 2	1 0	20.49 20.89
4.023	40	1	0	1	22.08
3.880 3.700	25 6	-1 1	1 2	1 0	22.90 24.03
3.435	100	2	1	0	25.92
3.244 3.042	20 19	0 -1	2	1	27.47 29.34
2.919	8	1	2	1	30.60
2.817 2.738	25 13	2	2 1	0	31.74 32.68
2.651	10	1	3	0	33.78
2.530	35	-2	2	1	35.45
2.515 2.468	30 45	0	0 3	2	35.67 36.37
2.404	20	3	1	0	37.38
2.391 2.376	8 2	2 -1	2	1	37.59 37.84
2.376	2	-1	1	2	38.19
2.327	2	-3	Ō	1	38.66
2.316	8	1	3	1	38.86
2.245 2.181	10 2	-3 -2	1 0	1 2	40.14 41.37
2.168 2.164	4 2	3	0 2	1 2	41.62 41.71
2.124M	13	ő	4	0	42.52
2.124M	0.0	-1	2	2	42.52
2.105	20	-2	3	1	42.92
2.101 2.040M	20 18	3 -3	1 2	1	43.02 44.37
2.040M		1	2	2	44.37
2.012 1.9570M	3 2	2 0	0 4	2	45.03 46.36
1.9570M		2	1	2	46.36
1.9392 1.9322	4 2	-2 3	2	2	46.81 46.99
1.9322	4	- 1	4	1	47.56
1.8799+	5	0	3	2	48.38
1.8799+ 1.8766	4	4	0 3	0	48.38 48.47
1.8536	14	-1	3	2	49.11
1.8497 1.8176	8 7	2 2	2	0 2	49.22 50.15
1.8149	4	-3	1	2	50.23
1.7975M 1.7975M	4	-3 1	3	1 2	50.75 50.75
1.7743	14	-4	1	1	51.46
1.7613	4	-2	4	1	51.87

Zinc Phosphate, γ -Zn₃(PO₄)₂ - (continued)

d(Å)	I	h	ıkl		2Θ(°)
1.7197	2	4	2	0	53.22
1.7029	6	-3	2	2	53.79
1.6792	6	4	1	1	54.61
1.6691M	12	3	1	2	54.97
1.6691M		-4	2	1	54.97
1.6579	6	1	5	0	55.37
1.6368	5	-1	1	3	56.15
1.6063M	2	1	0	3	57.31
1.6063M		-1	4	2	57.31
1.5881	1	4	2	1	58.03
1.5667M	5	4	3	0	58.90
1.5667M		1	5	1	58.90
1.5595	10	0	2	3	59.20
1.5545	12	-3	3	2	59.41
1.5493	10	2	5	0.	59.63

CAS registry no. 7543-51-3
Sample The sample was a reagent from the Chicago Apparatus Co., recrystallized from aqueous solution.
Color Colorless
Structure Orthorhombic, Pnma (62), Z = 4. The structure of hopeite has been determined by Mamedov et al. [1961] and Liebau [1965].
Lattice constants of this sample
$a = 10.611(1) \stackrel{\circ}{A}$ b = 18.312(2) c = 5.0309(6)
a/b = 0.5795 c/b = 0.2747
Volume o 977.55 A ³
Density (calculated) 3.113 g/cm ³
Figure of merit F ₃₀ = 73.8(0.010,40)
Polymorphism A polymorph of Zn ₃ (PO ₄) ₂ ·4H ₂ O is called parahopeite [Chao, 1969]. The pattern for parahopeite is on card 24-1461.
Additional patterns 1. PDF card 1-964 [Hanawalt et al., 1938] 2. PDF card 9-497 [Murdoch, Univ. of Cal., Los Angeles, Calif.], natural mineral. 3. PDF card 23-747 [Komrska and Satava 1969] 4. PDF card 26-1397 [Whitaker, 1973], natural mineral
References Chao, G. Y. (1969). Z. Kristallogr, Kristallgeometrie Kristallphys. Kristallchem. 130, 261. Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457. Komrska, J. and Satava, V. (1969). Silikaty
<pre>13, 135. Liebau, F. (1965). Acta Crystallogr. 18, 352. Mamedov, C. S., Gamidov, R., and Belov, N. W.</pre>
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CuKα ₁ λ	= 1.540598	o A;	tem	p. 2	.5±1 °C
Internal	standard	W, a	=	3.16	524 Å
d(A)	I	1	hkl		2Θ(°)
9.16 5.311 5.095 4.855 4.576	55 17 25 30 55	0 2 2 0 0	2 0 1 1 4	0 0 0 1 0	9.65 16.68 17.39 18.26 19.38
4.414 4.072 4.005 3.880 3.648M	35 7 20 14 9	1 1 2 0 2	1 2 3 3 0	1 1 0 1	20.10 21.81 22.18 22.90 24.38
3.648M 3.468 3.391 3.225 3.134	30 40 1 9	1 2 2 1 2	3 4 2 4 3	1 0 1 1	24.38 25.67 26.26 27.64 28.46
3.053 3.015 2.963 2.855+ 2.855+	1 4 8 100	0 2 0 3 2	6 5 5 1 4	0 0 1 1	29.23 29.61 30.14 31.30 31.30
2.760 2.652 2.614 2.585 2.548	3 19 25 3 15	3 4 3 2 4	2 0 3 5 2	1 0 1 1 0	32.41 33.77 34.28 34.67 35.19
2.535 2.515 2.445M 2.445M 2.426M	11 15 3	1 0 1 3 1	6 0 0 4 1	1 2 2 1 2	35.38 35.67 36.72 36.72 37.02
2.426M 2.342 2.321 2.288 2.271M	7 1 7 15	0 2 0 0	2 6 7 8 3	2 1 1 0 2	37.02 38.40 38.77 39.35 39.66
2.271M 2.268 2.206M 2.206M 2.190	13 4 2	3 1 2 0 4	5 7 2 4 3	1 1 2 2 1	39.66 39.71 40.88 40.88 41.18
2.158 2.148 2.130 2.100M 2.100M	7 3 1 11	1 4 2 2 3	4 5 3 8 6	2 0 2 0 1	41.83 42.02 42.41 43.03 43.03
2.038M 2.038M 2.002M 2.002M 1.977	3 16 2	3 2 4 3 4	1 4 6 2 5	2 2 0 2 1	44.42 44.42 45.26 45.26 45.87

Zinc Phosphate Hydrate (Hopeite), $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ - (continued)

d(A)	I	hkl	2θ(°)
1.940+	25	3 7 1	46.79
1.940+		2 8 1	46.79
1.9111	2	5 2 1	47.54
1.8994	1	2. 9 0	47.85
1.8715	1	3 4 2	48.61
1.8618M	2	4 7 0	48.88
1.8618M		5 3 1	48.88
1.8247	15	4 0 2	49.94
1.7985	1	5 4 1	50.72
1.7896M	1	4 2 2	50.99
1.7896M		3 5 2	50.99
1.7772	3	2 9 1	51.37
1.7361	5	6 2 0	52.68
1.7306	4	2 10 0	52.86
1.7252	3	5 5 1	53.04
1.7014	2	3 6 2	53.84
		_	
1.6953	6	4 4 2	54.05
1.6719	6	1 8 2	54.87
1.6646	5	3 9 1	55.13
1.6370	5	2 10 1	56.14
1.6298	3	1 2 3	56.41
1.6169	3	0 3 3	56.90
1.6143M	4	490	57.00
1.6143M		3 7 2	57.00
1.5974	4	5 2 2	57.66
1.5931M	4	2 1 3	57.83
1.5931M		6 5 0	57.83
1.5755M	1	2 2 3	58.54
1.5672+	10	5 3 2	58.88
1.5672+		6 4 1	58.88
1.5633	9	1 11 1	59.04
1.5295M	ģ	6 6 0	60.48
1.5295M		5 4 2	60.48
	10		60.66
1.5254M	10	0 12 0	
1.5254M		0 5 3	60.66
1.5161M	3	2 9 2	61.07
1.5161M		3 0 3	61.07
1.5092M	10	2 4 3	61.38
1.5092M		1 5 3	61.38
1.5068	7	4 10 0	61.49

Structure

Monoclinic, C2/m (12), Z = 2. The structure was determined by Moore and Araki [1976], for a sample from Serra de Mangabeira, Bahia, Brazil.

Atom positions

2(a)	1.8 antimony and 0.2 iron
4(g)	4 antimony
2(d)	2 aluminum
8(j)	7.52 aluminum and 0.48 iron
8(j)	8 oxygen in each of 3 different sites
4(i)	4 oxygen in each of 2 different sites
The sir	ngle crystal analysis did not refine
positio	ons for the Al atoms in the tetrahedral
sites a	and they were omitted also from calcula-
tion of	this powder pattern. Minor amounts of
W ⁺⁶ in	the octahedral sites were not deter-
mined e	either but their contribution was
absorbe	ed into the site distribution refine-

Lattice constants

ment [Moore and Araki, 1976].

a	=	9.407(6)	A
b	=	11.542(8)	
С	=	4.410(3)	
В	=	90.94(3)°	

a/b = 0.8150c/b = 0.3821

(published values: a = 9.406(6) Å, b = 11.541(8), c = 4.410(3), $\beta = 90.94(3)$ ° [Moore and Araki, 1976]).

Volume 6 478.75 A³

Density

(calculated) 5.362 g/cm³
This is the value calculated from the formula above, based on a chemical analysis by Moore and Araki in their table 1 part A [1976]. Due to the problems in the site distribution, mentioned above, a density is different if calculated from the multiplicities given in the atom positions.

Thermal parameters

Isotropic [Moore and Araki, 1976]

Scattering factors

Al³⁺, Fe³⁺, O¹⁻, Sb⁵⁺ [Cromer and Mann, 1968]. Dispersion corrections were applied to Al, Fe, and O [Cromer and Liberman, 1970].

Scale factors (integrated intensities) $\gamma = 0.1911 \times 10^{-3}$

 $\gamma = 0.1911 \times 10^{-6}$ $I/I_{corundum}$ (calculated) = 1.74 for reflection with $hk\ell = \overline{2}01$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u>, 321. Cromer, D. T. and Liberman, D. J. (1970). J. Chem. Phys. <u>53</u>, 1891. Moore, P. B. and Araki, T. (1976). Neues Jahrb. Mineral. Abh. 126, 113.

	ulated	Pattern	(Pe	ak	heights)
d(A)	I		hkl		2Θ(°) λ - 1.540598A
7.28	27	1	1	0	12.14
5.76	18	0	2	0	15.36
4.70	84	2	0	0	18.86
4.41	40	0	0	1	20.14
3.792	21	-1	1	1	23.44
3.751	18	1	1	1	23.70
3.645	10	2	2	0	24.40
3.559	30	1	3	0	25.00
3.504	25	0	2	1	25.40
3.243	100	-2	0	1	27.48
3.191	99	2	0	1	27.94
3.026	2	3	1	0	29.50
2.884	21	0	4	0	30.98
2.827	17	- 2	2	1	31.62
2.778	37	-1	3	1	32.20
2.763	33	1	3	1	32.38
2.513	10	-3	1	1	35.70
2.4755	10	3	1	1	36.26
2.4597	53	2	4	0	36.50
2.4302	19	3	3	0	36.96
2.4138	57	0	4	1	37.22
2.3517	21	4	0	0	38.24
2.2047	11	0	0	2	40.90
2.1772	5	4	2	0	41.44
2.1553	49	-2	4	1	41.88
2.1397	19	- 3	3	1	42.20
2.1168	10	3	3	1	42.68
2.1027	3	1	1	2	42.98
2.0607	24	4	0	1	43.90
2.0087	5	-2	0	2	45.10
1.9837	13	2	0	2	45.70
1.9642	4	-4		1	46.18
1.9404	4	4	2	1	46.78
1.8968	2	-2		2	47.92
1.8799	7	-1	3	2	48.38
1.8755	6	2	2	2	48.50
1.8697	5	1	3	2	48.66
1.8568	2	5	1	0	49.02
1.8227	11	4	4	0	50.00
1.7802	1	2	6	0	51.28
1.7629	2	0	6	1	51.82
1.7515	9	0	4	2	52.18
1.7209	1	- 5	1	1	53.18
1.6921	24	-4	4	1	54.16
1.6772	23	4	4	1	54.68

			٠.		
d(A)	I	h	ıkl		2Θ(°) λ - 1.540598Å
1.6489 1.6349	34	-2 2	4	2 2	55.70
1.6216	37 31	-4	4 0	2+	56.22 56.72
1.5954 1.5859	17 8	4 -5	0	2 1	57.74 58.12
	_	_	_		51.52
1.5701 1.5672	9 8	5 6	3	1 0	58.76 58.88
1.5378 1.5254	1 10	4 -1	7	2	60.12 60.66
1.5222	13	1	7	1	60.80
1.5132	1	6	2	0	61.20
1.4848	7 8	- 6 6	0	1 1+	62.50 63.22
1.4593	5	3	7	0+	63.72
1.4428	12	0	8	0	64.54

	Calculated	Patter	'n	(In	tegrated)
d(A)	I	h	kℓ	,	2Θ(°) ° λ - 1.540598A
7.29 5.77 4.70 4.41 3.795 3.752 3.646 3.561	23 16 78 38 20 16 9	1 0 2 0 -1 1 2	1 2 0 0 1 1 2 3	0 0 0 1 1 1	12.13 15.34 18.85 20.12 23.43 23.69 24.40 24.99
3.504 3.243 3.191 3.026 2.885 2.827 2.792	24 100 100 2 . 21 17 14	0 -2 2 3 0 -2 2	2 0 0 1 4 2 2	1 1 0 0 1 1	25.40 27.48 27.94 29.50 30.97 31.62 32.03
2.779 2.762 2.513 2.4765 2.4595	33 29 10 7 57	-1 1 -3 3 2	3 3 1 1 4	1 1 1 1 0	32.19 32.39 35.69 36.24 36.50
2.4304 2.4145 2.3514 2.2047 2.1776	15 61 23 12 3	3 0 4 0 4	3 4 0 0 2	0 1 0 2 0	36.96 37.21 38.24 40.90 41.43
2.1558 2.1401 2.1400 2.1178 2.1172	54 1 17 1 10	-2 2 -3 -1 3	4 3 1 3	1 1 1 2 1	41.87 42.19 42.19 42.66 42.67

d(A)	I		hkl		2Θ(°) λ - 1.540 5 98Å
2.1029 2.0609 2.0595 2.0089 1.9838	2 24 3 5 14	1 4 0 -2 2	1 0 2 0 0	2 1 2 2 2	42.97 43.90 43.93 45.09 45.70
1.9644 1.9408 1.8973 1.8797	5 4 2 7 1	-4 4 -2 -1 2	2 2 2 3 2	1 1 2 2 2	46.17 46.77 47.91 48.38 48.49
1.8693 1.8566 1.8228 1.7805 1.7632	5 1 13 1 2	1 5 4 2 0	3 1 4 6 6	2 0 0 0 1	48.67 49.02 50.00 51.27 51.81
1.7519 1.7211 1.7013 1.6922 1.6900	26	0 -5 5 -4 5	4 1 1 4 3	2 1 1 1 0	52.17 53.17 53.84 54.16 54.23
1.6770 1.6487 1.6474 1.6434	38 1 5	4 -2 2 -3 2	4 4 6 3 4	1 2 1 2 2	54.69 55.71 55.75 55.90 56.23
1.6241 1.6227 1.6217 1.5953 1.5859	25 20	1 3 -4 4 -5	7 3 0 0 3	0 2 2 2 2	56.63 56.68 56.72 57.74 58.12
1.5703 1.5689 1.5676 1.5612 1.5377	1 5 1	5 1 6 -4 4	3 5 0 2 2	1 2 0 2 2	58.75 58.81 58.86 59.13 60.13
1.5254 1.5226 1.5128 1.4848 1.4698	10 1 8	-1 1 6 -6 0	7 7 2 0 0	1 1 0 1 3	60.66 60.78 61.22 62.50 63.21
1.4695 1.4593 1.4583 1.4444 1.4427	5 1 1	6 3 5 -1 0	0 7 5 1 8	1 0 0 3 0	63.23 63.72 63.77 64.46 64.54
1.4379	2	-6	2	1	64.78

Structure Monoclinic, P2 ₁ /m (11), Z = 2. The structure was determined by Moore and Araki [1976] using data from sample #C4430, U.S. National Museum. The original location was Diamantina, Minas Gerais, Brazil.
Atom positions Moore and Araki [1976]
2(e) 2 antimony 2(e) 2 titanium 4(f) 1.72 iron and 2.28 titanium 4(f) 1.72 titanium and 2.28 iron 2(e) 2 oxygen 2(e) 2 hydroxyl 4(f) 4 oxygen in each of 6 different sites 4(f) 4 iron
Lattice constants
a = 7.160(1) A b = 14.348(3) c = 4.970(1) $\beta = 104.61(2)^{\circ}$
a/b = 0.4990 c/b = 0.3464
(published values: $a = 7.160(1) \text{ Å}$, $b = 14.347(3)$, $c = 4.970(1)$, $\beta = 104.61(2)^{\circ}$ [Moore and Araki, 1976]).
Volume • 494.1 A ³
Density (calculated) 4.798 g/cm ³
Thermal parameters Isotropic [Moore and Araki, 1976]
Scattering factors Sb ³⁺ , Fe ³⁺ , Ti ⁴⁺ , O ⁻ [Cromer and Mann, 1968]. Antimony, iron and titanium factors were corrected for dispersion [Cromer and Liberman, 1970].
Scale factors (integrated intensities) $ \gamma = 0.1340 \times 10^{-3} $ I/I corundum (calculated) = 1.58 for reflection with hk ℓ = 131.
References Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u> , 321. Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. <u>53</u> , 1891. Moore, P. B. and Araki, T. (1976). Neues Jahrb. Mineral. Abh. <u>126</u> , 292.

	culated Pa	ttern	(Pe	ak he	eights)	
d(Å)	I	1	hkl	γ	20(°) \ - 1.54 0 598	s A
6.23	21	1	1	0	14.20	
4.98	5	1	2	0	17.80	
4.81	21	0	0	1	18.44	
4.52	18	-1	0	1	19.64	
4.31	5	-1	1	1	20.60	
3.994	26	0	2	1	22.24	
3.935	7	1	3	0	22.58	
3.824	25	-1	2	1	23.24	
3.584	3	0	4	0	24.82	
3.553	5	1	0	1	25.04	
3.461	4	2	0	0	25.72	
3.453	4	1	1	1	25.78	
3.366	16	2	1	0	26.46	
3.222	8	-2	0	1	27.66	
3.184	37	1	4	0+	28.00	
3.119	50	2	2	0	28.60	
2.940	10	-2	2	1	30.38	
2.852	100	1	3	1	31.34	
2.808	19	-1	4	1+	31.84	
2.673	90	-2	3	1	33.50	
2.524	4	1	4	1	35.54	
2.486	13	2	1	1	36.10	
2.473	34	-1	0	2	36.30	
2.468	29	0	5	1	36.38	
2.423	5	-1	5	1	37.08	
2.391	16	0	6	0	37.58	
2.372	4	0	1	2	37.90	
2.338	2	- 1	2	2	38.48	
2.309	3	3	0	0	38.98	
2.293	8	-3	1	1	39.26	
2.280	8	3	1	0+	39.50	
2.260	6	1	6	0	39.86	
2.232	21	1	5	1	40.38	
2.210	5	2	5	0+	40.80	
2.199	3	3	2	0	41.02	
2.143	13	-2	5	1+	42.14	
2.113	7	1	0	2+	42.76	
2.090	7	1	1	2+	43.26	
2.080	5	3	3	0	43.48	
2.027	15	1	2	2	44.68	
1.997	8	0	4	2	45.38	
1.984	2	1	6	1	45.70	
1.966	2	1	7	0	46.14	
1.942	2	3	4	0	46.74	
1.932	3	1	3	2	47.00	
1.926	8	-3	0	2	47.16	
1.921	7	-2	6	1	47.28	
1.913	9	-2	4	2+	47.50	
1.8953	3	2	5	1	47.96	
1.8865	6	3	1	1+	48.20	

-			
d(Å)	I	hkl	2Θ(°) 。 λ - 1.540598A
			Λ - 1.340396A
1.8604	9	-3 2 2	48.92
1.8427	2	0 5 2	49.42
1.8051	5	- 3 5 1	50.52
1.7998	6	3 5 0	50.68
1.7763	15	2 0 2	
1.7641	8	-4 1 1·	
1.7361	3	1 8 0	52.68
1.7294	5	-2 7 1	52.90
1.7246	5	2 2 2	53.06
1.7191	16	-1 6 2	+ 53.24
1.7014	2	1 5 2	53.84
1.6967	2	0 6 2	54.00
1.6806	2	0 8 1	54.56
1.6665	6	2 3 2	
1.6615	7	3 6 0	55.24
1.0015	,	3 0 0	33.24
1.6571	4	-1 0 3	55.40
1.6424	6	- 2 6 2	55.94
1.6285	2	4 3 0	56.46
1.6112	10	-4 0 2	57.12
1.6010	4	-4 1 2	
1.5924	17	2 8 0	57.86
1.5859	28	3 5 1	58.12
1.5721	3	-4 2 2	58.68
1.5672	3	-2 8 1	58.88
1.5648	4	-1 3 3	+ 58.98
1.5600	4	4 4 0	± 50 10
1.5369	4		
	5	-3 7 1 -2 3 3	
1.5332 1.5272	3		
1.5200	12	0 3 3	60.90
1.5119	20	- 4 5 1	+ 61.26
1.5039	6	4 1 1	
1.5004	4	-3 6 2	
1.4887	3	3 0 2	
1.4831	2	4 5 0	
1.4802	2	4 2 1	+ 62.72
	2		
1.4743	6	1 1 3	
1.4709	5	1 7 2	
1.4544	2	1 9 1	
1.4420	3	4 3 1	64.58
1.4344	24	- 1 5 3	+ 64.96
1.4239	5	-5 1 1	
1.4208	3	3 3 2	
1.4098	2	-2 5 3	
1.4049	5	-2 8 2	
1 /0-5	_		
1.4015	3	0 5 3	66.68

	Calculated	Pattern	(Int	egrated)	
d(A)	I	h	ıkl	2Θ(°) ° λ - 1.540598A	
6.24 4.98 4.81 4.52 4.31	18 4 18 16 4	1 1 0 -1 -1	1 0 2 0 0 1 0 1 1 1	17.78 18.43 19.62	
3.995 3.936 3.825 3.587 3.553	6 6 5 24 7 3	0 1 -1 0 1	2 1 3 0 2 1 4 0 0 1	22.57 23.24 24.80	
3.464 3.449 3.393 3.363 3.223	9 2 1 3 7 15	2 1 0 2 -2	0 0 1 1 3 1 1 0 0 1	25.81 26.26 26.45	
3.185 3.184 3.120 2.940 2.875	4 10 0 49 0 10	1 1 2 -2 0	4 (2 1 2 (2 1 4 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	28.00 28.59 30.38	
2.852 2.810 2.800 2.673 2.653	0 14 6 4 3 94	1 -1 2 -2 1	3 1 4 1 3 0 3 1 5 0	31.82 31.87 33.50	
2.524 2.48 2.47 2.464 2.423	7 10 3 32 4 11	1 2 -1 0 -1	4 1 1 0 2 5 1 5 1 5	36.09 2 36.30 1 36.43	
2.39 2.39 2.37 2.33 2.30	1 14 2 3 8 2	-2 0 0 -1 3	4 1 6 0 1 2 2 2 0 0	37.58 2 37.91 2 38.47	
2.293 2.286 2.266 2.266	0 6 0 2 0 5	-3 3 0 1 -2	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	39.49 2 39.49 39.85	
2.233 2.210 2.210 2.190 2.140	0 1 0 3 8 2	1 -3 2 3 0	5 1 2 1 5 0 2 0 3 2	40.80 40.80 41.02	
2.14 2.14 2.11 2.11 2.09	1 3 4 3 3 4	-2 0 -1 1	5 1 6 1 6 1 0 2 1 2	42.17 42.74 2 42.77	

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
2.090	3	-3 3 1	43.26
2.080	4	3 3 0	43.48
2.036	1	-1 4 2	44.46
2.027	17	1 2 2	44.68
1.997	8	0 4 2	45.37
1.984	2	1 6 1	45.69
1.966	2	1 7 0	46.15
1.942	1	3 4 0	46.74
1.932	2	1 3 2	46.98
1.926	8	-3 0 2	47.15
1.920	2	-2 6 1	47.30
1.912	8	-2 4 2	47.51
1.909	3	-3 1 2	47.60
1.8957	2	2 5 1	47.95
1.8865	5	3 1 1	48.20
1.8856	2	0 7 1	48.22
1.8668	1	-1 7 1	48.74
1.8601	9	-3 2 2	48.93
1.8431	1	0 5 2	49.41
1.8056	5	-3 5 1	50.51
1.7992	5	3 5 0	50.70
1.7766	14	2 0 2	51.39
1.7755	3	1 7 1	51.42
1.7682	1	3 3 1	51.65
1.7655	4	-4 1 1	51.74
1.7641	2	2 7 0	51.78
1.7631	3	2 1 2	51.81
1.7363	3	1 8 0	52.67
1.7321	1	4 0 0	52.81
1.7295	4	-2 7 1	52.90
1.7245	1	2 2 2	53.06
1.7196	2	4 1 0	53.22
1.7191	15	-1 6 2	53.24
1.7013	2	1 5 2	53.84
1.6956	1	0 6 2	54.04
1.6805	2	0 8 1	54.57
1.6674	2	-4 3 1	55.03
1.6671	2	-1 8 1	55.04
1.6654	2	2 3 2	55.10
1.6612	5	3 6 0	55.25
1.6563 1.6427 1.6286 1.6138 1.6114	1 7 1 1	-1 0 3 -2 6 2 4 3 0 -1 2 3 -4 0 2	55.43 55.93 56.46 57.02 57.11
1.6013	2	-4 1 2	57.51
1.6011	1	1 8 1	57.52
1.5927	17	2 8 0	57.85
1.5914	1	2 7 1	57.90
1.5859	29	3 5 1	58.12

0					
d(A)	I	h	kl		20(°)
					λ - 1.540598Α
1.5791	2	-2	2	3	58.39
1.5722	2	-4	2	2	58.67
1.5672	2	-2	8	1	58.88
1.5651	2	-1	3	3	58.97
1.5599	1	0	7	2	59.18
1.5598	1	4	4	0	59.19
1.5370	4	-3	7	1	60.16
1.5333	2	-2	3	3	60.31
1.5330	1	3	7	0	60.33
1.5270	1	-4	3	2	60.59
1 5200	12	0	2	2	60.90
1.5200	13	0 0	3 9	3 1	61.20
1.5132	20	-4	5	1	
1.5120 1.5105	20	-4 2	5 5	2	61.26 61.32
	2 2	4	о 1	1	61.61
1.5042	Z	4	1	1	01.01
1.5037	1	-1	4	3	61.63
1.5035	1	-1	9	1	61.64
1.4886	3	3	0	2	62.32
1.4829	1	4	5	0	62.59
1.4800	1	4	2	1	62.73
1.4755	3	-2	4	3	62.94
1.4748	1	-3	2	3	62.98
1.4741	4	1	1	3	63.01
1.4711	1	1	7	2	63.15
1.4699	1	-4	4	2	63.21
1.4545	1	1	9	1	63.96
1.4519	1	-1	8	2	64.08
1.4421	2	4	3	1	64.57
1.4373	9	-3	3	3	64.81
1.43/3	11		0 .	0	64.94
1.7570				,	
1.4345	14	-1	5	3	64.96
1.4261	1	2	6	2	65.39
1.4240	4	- 5	1	1	65.50
1.4214	1	3	3	2	65.63
1.4099	2	-2	5	3	66.23
1.4050	2	-4	5	2	66.49
1.4050	2	-2	8	2	66.50
1.4036	1	- 3	7	2	66.57
1.3995	1	0	5	3	66.79

1. 2-Diethylaminoethyl benzilate hydrochloride
Structure Triclinic, $P\overline{1}$ (2), $Z = 2$. The structure was refined by Petcher et al. [1974].
Atom positions All atoms were in general positions 2(i).
Lattice constants
a = $8.792(4)$ Å b = $15.949(8)$ c = $7.091(6)$ α = $95.73(1)^{\circ}$ β = $94.10(1)$ γ = $87.57(1)$
a/b = 0.5513 c/b = 0.4446
(published values: $a = 879.1(4)$ pm, $b = 1594.8(8)$, $c = 709.1(6)$, $\alpha = 95.73(1)^{\circ}$, $\beta = 94.10(1)$, $\gamma = 87.57(1)$ [Petcher et al., 1974])
Volume o 986.2 A ³
Density (calculated) 1.225 g/cm ³
Thormal noremeters
Thermal parameters Isotropic. For hydrogen atoms, overall $B = 5.5$. For all other atoms, isotropic B_i were estimated from β_{ij} for individual atoms.
Isotropic. For hydrogen atoms, overall B = 5.5. For all other atoms, isotropic B.
Isotropic. For hydrogen atoms, overall B = 5.5. For all other atoms, isotropic B, were estimated from β_{ij} for individual atoms. Scattering factors
Isotropic. For hydrogen atoms, overall B = 5.5. For all other atoms, isotropic B, were estimated from β_{ij} for individual atoms. Scattering factors Zero ionization [International Tables, 1962] Scale factors (integrated intensities) $\gamma = 0.3987 \times 10^{-3}$ I/I corundum (calculated) = 0.380 for reflection

Ca	lculated	Pattern	(Pea	ık hei	ghts)
d(A)	I		hkl	λ	2Θ(°) - 1.540598A
15.83 8.75 7.91 7.78 7.56	40 60 4 13 14	0 1 0 1 -1	1 0 2 1 1	0 0 0 0	5.58 10.10 11.18 11.36 11.70
7.03 6.67 6.21 5.77 5.53	8 39 3 48 100	0 0 0 -1 0	0 -1 1 2 -2	1 1 1 0 1+	12.58 13.26 14.26 15.34 16.02
5.29 5.02 4.96 4.85 4.52	14 2 1 4 2	0 0 1 -1	3 2 1 -2 -2	0 · · · · · · · · · · · · · · · · · · ·	16.76 17.64 17.86 18.26 19.62
4.454 4.410 4.312 4.263 4.184	7 7 24 10 2	-1 -1 1 2 -2	3 2 2 1 1	0 1 1 0 0	19.92 20.12 20.58 20.82 21.22
4.081 4.044 3.962 3.890 3.844	4 1 3 3 8	-1 0 0 2 1	-3 3 4 2 -3	1 1 0 0	21.76 21.96 22.42 22.84 23.12
3.776 3.657 3.610 3.573 3.509	43 37 6 6 26	-2 1 2 -2 0	2 4 0 -2 -1	0 0+ 1+ 1 2+	23.54 24.32 24.64 24.90 25.36
3.432 3.341 3.314 3.262 3.236	6 21 19 3 3	2 -2 0 2 -2	3 2 4 2 -3	0 1+ 1+ 1	25.94 26.66 26.88 27.32 27.54
3.204 3.175 3.102 3.010 3.006	9 4 11 8 8	-1 1 1 2 0	-2 -1 4 -3 -5	2+ 2 1+ 1	27.82 28.08 28.76 29.66 29.70
2.974 2.921 2.888 2.854 2.807	1 1 4 4 2	-1 3 3 -3 0	-3 0 1 1 3	2+ 0 0+ 0 2	30.02 30.58 30.94 31.32 31.86
2.764 2.746 2.701 2.670 2.665	4 12 2 3 3	-3 -2 -1 -3	0 1 -4 -2 5	1+ 2 2+ 1 1+	32.36 32.58 33.14 33.54 33.60

d(A)	I	hkl	2Θ(°) λ - 1.540598A
2.644	3	2 4 1+	33.88
2.614	3	2 5 0	34.28
2.598	3	2 1 2+	34.50
2.583	6	1 -4 2	34.70
2.553	3	-3 2 1+	35.12
2.527	2	-2 5 0	35.50
2.505	3	-1 6 0+	35.82
2.481	2	2 2 2+	36.18
2.433	1	-1 -5 2+	36.92
2.399	3	0 6 1+	37.46
2.393	3	3 4 0	37.56
2.362	3	3 -3 1	38.06
2.355	3	0 -1 3+	38.18
2.349	3	-2 5 1+	38.28
2.340	2	1 -5 2	38.44
2.326 2.312 2.300 2.263 2.229	2 3 2 1	2 3 2+ -3 4 0 2 6 0 2 -4 2+ 1 0 3+	38.68 38.92 39.14 39.80 40.44
2.221	1	0 -7 1+	40.58
2.213	1	1 7 0	40.74
2.190	3	4 0 0+	41.18
2.181	4	-1 -7 1+	41.36
2.170	3	1 5 2	41.58
2.154	1	2 -6 1+	41.90
2.140	1	-2 -1 3	42.20
2.132	2	4 2 0+	42.36
2.112	2	-3 5 0+	42.78
2.101	1	1 2 3+	43.02
2.094 2.060 2.041 2.037 2.033	1 2 2 2 2 2	-4 2 0+ -3 3 2 2 7 0+ 3 -3 2+ 3 -5 1	43.16 43.92 44.34 44.44 44.54
2.023	2	3 5 1+	44.76
2.017	2	1 -4 3+	44.90
2.014	1	2 -1 3+	44.98
1.995	1	1 3 3+	45.42
1.987	2	2 5 2+	45.62
1.975	1	-1 -7 2+	45.90
1.965	2	-3 -5 2+	46.16
1.924	1	2 -3 3+	47.20
1.919	1	1 -7 2+	47.34
1.901	3	2 7 1+	47.80
1.830	2	-4 4 1+	49.78
1.826	2	1 8 1+	49.90
1.820	1	4 -4 1	50.08
1.804	2	0 5 3+	50.56
1.800	2	-3 2 3	50.66

d(Å)	Ι	hkl λ	20(°) - 1.540598A
1.768	1	2 -7 2+	51.66
1.760	2	0 0 4+	51.92
1.757	2	-4 3 2+	52.00
1.750	2	0 -9 1+	52.22
1.723	1	2 8 1+	53.10
1.714	1	-4 -6 1+	53.40
1.709	1	3 -6 2+	53.58
1.699	1	1 -9 1+	53.92
1.655	1	-4 -2 3+	55.48
1.619	1	-3 -6 3+	56.84
1.584	1	4 -5 2+	58.20

	Calculated	Patter	n	(Int	egrated)
d(A)	I		hk	Q.	2Θ(°) ° λ - 1.540598A
15.86	66	0	1	0	5.57
8.76	100	1	0	0	10.08
7.93	4	0	2	0	11.15
7.79	20	1	1	0	11.35
7.56	23	-1	1	0	11.70
7.04	13	0	0	1	12.56
6.68	66	0	-1	1	13.25
6.21	5	0	1	1	14.24
5.78	83	- 1	2	0	15.32
5.68	1	-1	0	1	15.59
5.54	94	0	-2	1	15.99
5.53	87	-1	-1	1	16.02
5.29	24	0	3	0	16.76
5.03	3	0	2	1	17.63
4.96	1	1	1	1	17.86
4.86	6	-1	-2	1	18.25
4.52	2	1	-2	1	19.60
4.457	11	-1	3	0	19.90
4.410	11	-1	2	1	20.12
4.313	43	1	2	1	20.58
4.263	14	2	1	0	20.82
4.186	2	-2	1	0	21.21
4.081	7	-1	-3	1	21.76
4.043	1	0	3	1	21.97
3.965	5	0	4	0	22.41
3.894	4	2	2	0	22.82
3.849	11	1	-3	1	23.09
3.838	3	-2	0	1	23.15
3.805	6	-2	-1	1	23.36
3.779	80	-2	2	0	23.52
3.687	21	-1	3	1	24.12
3.662	36	1	4	0	24.29
3.661	9	-2	1	1	24.29
3.655	. 27	1	3	1	24.33
3.612	4	2	0	1	24.63
3.012	,	-	J	1	24.03

d(A)	, I	hkl	2θ(°) λ - 1.540598A
3.608	4	0 -4	1 24.66
3.575	8	-2 -2	1 24.89
3.565	1		0 24.96
3.520	21		2 25.28
3.509	33	0 -1	2 25.36
3.434	- 9		0 25.92
3.418	1	-1 -4	1 26.05
3.368	15	0 1	2 26.45
3.346	20	-2 2	1 26.62
3.346	6	-1 -1	2 26.62
3.340	13		2 26.67
3.319	16		1 26.84
3.316	5	-2 3	0 26.86
3.313	14	2 -2	1 26.89
3.262	3	2 2	1 27.32
3.238	4	-2 -3	1 27.52
3.206	9	-1 - 2	2 27.80
3.205	7	-1 1	2 27.81
3.192	1	1 0	2 27.93
3.176	5	1 -1	2 28.07
3.107	2	0 2	2 28.71
3.106	4	-1 4	1 28.71
3.102	16	1 4	1 28.76
3.011	13	2 -3	1 29.64
3.003	6	0 -5	1 29.72
2.993	1	2 4	0 29.82
2.973	1		2 30.04
2.921	1		0 30.58
2.891	4		0 30.90
2.887	3	1 2	2 30.95
2.882	1	-2 -4	1 31.01
2.855	8		0 31.31
2.846	2		2 31.41
2.807	3		2 31.86
2.792	1	0 5	1 32.03
2.769	2	0 -4	2 32.30
2.765	2 4	-3 0	1 32.35
2.747	24	-2 1	2 32.57
2.702	2	-1 -4	2 33.13
2.698	1	2 -4	1 33.18
2.671	4	-3 -2	1 33.52
2.664	2	1 5	1 33.62
2.658	1	2 0	2 33.70
2.649	1	-2 4	1 33.81
2.643	2	2 4	1 33.89
2.636	2	3 0	1 33.98
2.614	5		0 34.28
2.599	2		2 34.48
	1	3 1	1 34.49
	1	2 I	1 34.47
2.598 2.596	1		0 34.52

	d(A)	I	hkl	2Θ(°) ° λ - 1.540598Å
	2.583 2.556 2.555 2.553 2.527	11 1 2 2 2 3	1 -4 2 1 6 0 -3 2 1 -2 -5 1 -2 5 0	34.70 35.08 35.10 35.13 35.49
	2.506	5	-1 6 0	35.80
	2.504	1	3 -2 1	35.83
	2.498	1	3 2 1	35.92
	2.482	2	2 2 2	36.17
	2.479	1	0 -5 2	36.21
	2.434	1	-1 -5 2	36.90
	2.433	1	-1 4 2	36.92
	2.408	2	2 -5 1	37.31
	2.400	2	1 4 2	37.44
	2.399	2	0 6 1	37.46
	2.393	4	3 4 0	37.56
	2.381	1	-3 3 1	37.75
	2.363	4	3 -3 1	38.05
	2.355	1	3 3 1	38.19
	2.355	2	0 -1 3	38.19
	2.350	2	-2 5 1	38.27
	2.346	1	0 0 3	38.33
	2.340	2	1 -5 2	38.44
	2.327	2	2 3 2	38.67
	2.327	1	-3 0 2	38.67
	2.313 2.300 2.262 2.229 2.220	5 3 1 2	-3 4 0 2 6 0 2 -4 2 1 0 3 0 -7 1	38.91 39.14 39.81 40.43 40.60
	2.213 2.193 2.191 2.189 2.182	2 2 2 2 2 3	1 7 0 0 2 3 4 0 0 -1 5 2 -1 -7 1	40.75 41.13 41.17 41.21 41.35
	2.181	2	4 1 0	41.37
	2.179	1	-3 2 2	41.41
	2.175	1	-1 7 0	41.49
	2.170	4	1 5 2	41.58
	2.166	1	3 -1 2	41.66
	2.154	1	2 -6 1	41.90
	2.140	1	-2 -1 3	42.19
	2.133	2	-4 0 1	42.33
	2.131	2	4 2 0	42.37
	2.113	1	-2 -2 3	42.76
	2.112	1	-3 5 0	42.79
	2.101	1	1 2 3	43.02
	2.060	3	-3 3 2	43.91
	2.046	1	1 7 1	44.23
	2.042	2	2 7 0	44.32
1				

Benactyzine Hydrochloride, $C_{20}H_{26}ClNO_3$ - (continued)

d(A)	I	hkl	2Θ(°) a
u(A)	1	IIKX	λ - 1.540598Å
2.037	2	3 -3 2	44.44
2.035	1	4 -1 1	44.49
2.032	1	3 - 5 1	44.56
2.023	2	3 5 1	44.76
2.014	1	2 -1 3	44.98
2.013	1	2 0 3	45.01
2.004	1	- 2 2 3	45.20
1.995	1	1 3 3	45.41
1.989	1	3 3 2	45.56
1.987	3	2 5 2	45.62
1.976	1	-1 -7 2	45.90
1.965	2	- 3 - 5 2	46.17
1.965	1	1 6 2	46.17
1.924	1	2 -3 3	47.19
1.919	1	-1 8 0	47.33
1.917	1	1 -7 2	47.39
1.907	1	- 2 3 3	47.66
1.902	1	-4 -2 2	47.77
1.902	4	2 7 1	47.79
1.900	2	1 -5 3	47.84
1.830	3	-4 4 1	49.77
1.819	1	4 -4 1	50.10
1.806	1	4 0 2	50.49
1.804	1	0 5 3	50.54
1.804	1	0 -8 2	50.56
1.800	2	- 3 2 3	50.66
1.770	1	2 -7 2	51.59
1.768	1	0 -1 4	51.66
1.760	2	0 0 4	51.92
1.757	1	- 4 3 2	52.00
1.750	1	0 -9 1	52.23
1.735	1	- 5 1 0	52.70
1.699	1	1 -9 1	53.92
1.619	1	-3 -6 3	56.83
1.588	1	-1 -8 3	58.04
1.584	1	4 -5 2	58.22

Structure

Monoclinic, C2/c (15), Z = 4. The structure was refined by Fanfani et al. [1975] using material from the U.S. National Museum of Natural History (NMNH #R17847) from Lavra da Ilha, Taquaral (Minas Gerais), Brazil.

Atom positions

Fanfani et al. [1975]

- 4(a) 2.68 aluminum with 1.32 positions void
- 4(e) 4 calcium
- 8(f) 5.6 magnesium plus 2.4 iron
- 8(f) 8 beryllium
- 8(f) 8 phosphorus
- 4(e) 4 phosphorus
- 8(f) 8 oxygen in each of 6 different sites
- 8(f) 8 hydroxyl
- 4(e) 4 hydroxyl
- 8(f) 8 water

Polymorphism

A triclinic roscherite exists and has a very similar atomic arrangement. Its chemical composition is somewhat different including the replacement of most of the magnesium by manganese [Fanfani et al., 1977].

Lattice constants

- a = 15.875(4) A
- b = 11.855(3)
- c = 6.605(1)
- $\beta = 95.35(3)^{\circ}$

a/b = 1.3391

c/b = 0.5571

(published values: a = 15.874(4) Å, b = 11.854(3), c = 6.605(1), $\beta = 95^{\circ}21'(2')$ [Fanfani et al., 1975]).

Volume 0 1237.6 Å³

120, 10 11

Density

(calculated) 2.768 g/cm³ (measured) 2.766(7) [Fanfani et al., 1975]

Thermal parameters

Isotropic [Fanfani et al., 1975]

Scattering factors

Zero ionization [International Tables, 1962].

Scale factors (integrated intensities)

 $\gamma = 0.1851 \times 10^{-3}$

 I/I_{corundum} (calculated) = 0.654 for reflection with hk ℓ = 110.

Additional patterns

1. PDF card 11-355 [Lindberg, 1958]. The data may represent a mixture of the monoclinic and triclinic forms.

References

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Lindberg, M. L. (1958). Amer. Mineral. <u>43</u>, 824.

Ca	lculated	Pattern	(Pea	ak h	neigl	nts)
d(A)	I		hkl		λ -	20(°) 。 1.540598A
9.48	100	1	1	0		9.32
7.89	3	2	0	0		11.20
5.925	83	0	2	0		14.94
5.549	2	-1	1	1		15.96
4.813	31	3	1	0		18.42
4.741	7	2	2	0		18.70
4.401	12	0	2	1		20.16
3.948	3	4	0	0+		22.50
3.831	1	1	3	0		23.20
3.736	4	3	1	1		23.80
3.343	29	-1	3	1		26.64
3.285	15	4	2	0+		27.12
3.160	51	3	3	0		28.22
3.142	46	-2	0	2		28.38
3.054	48	1	1	2+		29.22
2.940	37	2	0	2		30.38
2.915	6	-3	3	1		30.64
2.873	16	0	2	2		31.10
2.854	10	4	2	1		31.32
2.829	16	-3	1	2		31.60
2.774 2.701 2.679 2.633 2.587	58 3 4 41 3	2 0 5 6 -2	4 4 1 0 4	0 1 1 0		32.24 33.14 33.42 34.02 34.64
2.527 2.468 2.420 2.408 2.371	4 3 6 12 6	2 1 -4 6 4	4 3 2 2 4	1+ 2+ 2+ 0		35.50 36.38 37.12 37.32 37.92
2.345	9	1	5	0+		38.36
2.326	1	-6	2	1		38.68
2.271	6	-4	4	1		39.66
2.258	2	5	3	1		39.90
2.239	2	4	2	2		40.24
2.218	25	7	1	0+		40.64
2.202	13	0	4	2		40.96
2.162	17	-1	1	3+		41.74
2.157	12	-6	0	2+		41.84
2.087	2	2	4	2		43.32

Beryllium Calcium Iron Magnesium Aluminum Phosphate Hydroxide Hydrate, Roscherite, $Be_2Ca(Fe_{0.7}Mg_{0.7})_2Al_{0.67}(PO_4)_3(OH)_3\cdot 2H_2O$ - (continued)

d(A)	I	hkl	2Θ(°) λ - 1.540598A
2.062 2.056	2 3	-3 1 3 0 2 3	43.88 44.00
2.046	8	7 1 1	44.24
2.033	8 10	-2 2 3+ -6 2 2	44.52 44.68
2.021	10	-0 2 2	44.00
1.976	14	-4 4 2+	45.88
1.971	10	6 4 0	46.00
1.922	8	-1 5 2+	47.26
1.917 1.909	8 5	2 6 0 5 3 2	47.38 47.60
1.909	J	3 3 2	47.00
1.892	2	-4 2 3+	48.04
1.885	3	1 3 3	48.24
1.874	2	4 4 2+	48.54
1.868	4 3	6 2 2 -5 1 3	48.70 48.84
1.003	3	-5 1 5	40.04
1.846	1	-8 2 1	49.32
1.839	2	7 3 1+	49.54
1.796	2	5 5 1	50.80
1.776	5	3 5 2	51.42
1.767	11	-8 0 2+	51.68
1.763	8	0 4 3+	51.80
1.748	3	-2 4 3	52.30
1.743	7	- 6 4 2	52.44
1.739	4	9 1 0	52.58
1.710	2	5 1 3	53.56
1.694	9	0 6 2+	54.10
1.684	2	1 7 0+	54.44
1.673	1	-2 6 2	54.84
1.657	4	-4 4 3	55.42
1.644	21	8 4 0+	55.88
1.640	18	6 4 2+	56.04
1.635	12	-1 7 1+	56.20
1.628	5	1 7 1+	56.48
			56.62
1.612	2	-1 5 3+	57.08
1.605	6	9 3 0+	57.38
1.5904	3	1 5 3+	57.94
1.5804	5	6 6 0+	58.34
1.5696	3	8 2 2	58.78
1.5662	5	8 4 1+	58.92
1.5629	3	7 5 1	59.06
1.5561	2		59.34
	1		
1.51/3	4	3 1 4+	61.02
1.5052	2	-7 5 2+	61.56
1.4930	6	-9 3 2+	62.12
1.4802	1	9 1 2+	62.72
1.4043	3	-3 / 2	63.48
1.628 1.624 1.612 1.605 1.5904 1.5804 1.5765 1.5696 1.5662 1.5629 1.5561 1.5236 1.5173	5 3 2 6 3 5 3 3 5 3 2 1 4	6 4 2+ -1 7 1+ 1 7 1+ -8 4 1 -1 5 3+ 9 3 0+ 1 5 3+ 6 6 0+ -3 7 1 8 2 2 8 4 1+ 7 5 1 6 2 3+ -7 3 3 3 1 4+ -7 5 2+ -9 3 2+	56.04 56.20 56.48 56.62 57.08 57.38 57.94 58.34 58.50 58.78 58.92 59.06 59.34 60.74 61.02 61.56 62.12

d(Å)	Ι	hkl	2Θ(°) λ - 1.540598Å
1.4601	2	-2 6 3	63.68
1.4569	4	- 6 6 2+	63.84
1.4420	1	5 7 1	64.58
1.4352	6	-2 4 4+	64.92

	lculated	Pattern	(In	teg	rated)
d(Å)	I		hkl		2Θ(°) ο λ - 1.540598A
9.48	100	1	1	0	9.32
7.90	3	2	0	0	11.19
5.927	87	0	2	0	14.93
5.552	2	-1	1	1	15.95
4.815	33	3	1	0	18.41
4.742	5	2	2	0	18.70
4.403	13	0	2	1	20.15
3.953	1	-2	2	1	22.48
3.951	3	4	0	0	22.48
3.834	1	1	3	0	23.18
3.736	5	3	1	1	23.80
3.345	33	-1	3	1	26.63
3.288	5	0	0	2	27.10
3.288	9	4	2	0	27.10
3.280	4	1	3	1	27.17
3.162	8	-1	1	2	28.20
3.161	46	3	3	0	28.21
3.141	46	-2	0	2	28.39
3.054	22	5	1	0	29.21
3.054	34	1	1	2	29.22
3.037	3	-4	2	1	29.39
2.964	5	0	4	0	30.13
2.940	44	2	0	2	30.38
2.914	3	-3	3	1	30.66
2.875	16	0	2	2	31.08
2.871	3	- 5	1	1	31.13
2.854	9	4	2	1	31.32
2.830	17	-3	1	2	31.59
2.789	1	3	3	1	32.07
2.776	8	-2	2	2	32.22
2.775	63	2	4	0	32.23
2.702	3	0	4	1	33.13
2.680	4	5	1	1	33.41
2.634	49	6	0	0	34.00
2.634	2	2	2	2	34.01
2.614	2 2	3	1	2	34.28
2.587		-2	4	1	34.64
2.527	4	2	4	1	35.49
2.524	1	-1	3	2	35.54
2.469	1	5	3	0	36.37

d(A)	I	1	hkl		2Θ(°) ° λ - 1.540598A
2.468	3	1	3	2	36.37
2.421	4	-4	2	2	37.11
2.419	2	4	0	2	37.14
2.407	14	6	2	0	37.32
2.371	7	4	4	0	37.92
2.345 2.345 2.325 2.271 2.258	3 7 1 7 2	-3 1 -6 -4 5	3 5 2 4 3	2 0 1 1	38.35 38.36 38.69 39.65 39.90
2.240 2.218 2.218 2.218 2.218 2.201	1 11 16 4 13	4 -1 7 3 0	2 5 1 3 4	2 1 0 2 2	40.23 40.64 40.64 40.65 40.96
2.199	1	1	5	1	41.01
2.192	2	4	4	1	41.15
2.162	18	-1	1	3	41.74
2.162	2	3	5	0	41.74
2.156	1	-6	0	2	41.86
2.156	1	-2	4	2	41.87
2.144	1	5	1	2	42.12
2.087	2	2	4	2	43.31
2.062	1	-3	1	3	43.86
2.056	2	0	2	3	44.01
2.047	1	-5	3	2	44.21
2.046	8	7	1	1	44.24
2.034	7	-2	2	3	44.52
2.031	2	3	5	1	44.58
2.026	8	-6	2	2	44.68
1.976	13	-4	4	2	45.88
1.976	4	0	6	0	45.89
1.976	2	8	0	0	45.89
1.969	2	6	4	0	46.06
1.968	1	6	0	2	46.08
1.923	1	-6	4	1	47.22
1.922	4	-1	3	3	47.26
1.922	4	-1	5	2	47.26
1.917	4	2	6	0	47.39
1.909	4	5	3	2	47.61
1.897	1	5	5	0	47.92
1.893	1	-4	2	3	48.03
1.885	3	1	3	3	48.25
1.874	1	4	4	2	48.54
1.868	4	6	2	2	48.71
1.862	1	-5	1	3	48.87
1.846	1	-8	2	1	49.32
1.838	2	7	3	1	49.54
1.796	2	5	5	1	50.80
1.776	6	3	5	2	51.42

d(A)	I	hkl	2Θ(°) 。 λ - 1.540598Å
1.768	8	-8 0 2	51.66
1.767	5	4 6 0	51.68
1.762	2	0 4 3	51.83
1.762	1	8 2 1	51.85
1.748	3	-2 4 3	52.29
1.744	7	-6 4 2	52.43
1.737	2	9 1 0	52.64
1.709	2	5 1 3	53.57
1.694	5	-8 2 2	54.09
1.694	6	0 6 2	54.11
1.684	2	1 7 0	54.44
1.673	1	-2 6 2	54.85
1.656	5	-4 4 3	55.43
1.644	10	0 0 4	55.88
1.644	16	8 4 0	55.88
1.643	2	9 1 1	55.93
1.640	1	-2 0 4	56.01
1.640	2	2 6 2	56.03
1.640	4	6 4 2	56.04
1.636	1	-7 1 3	56.18
1.635	7	-1 7 1	56.21
1.628	2	8 0 2	56.48
1.627	2	1 7 1	56.50
1.625	1	-8 4 1	56.60
1.612	1	-1 5 3	57.07
1.605	2	1 1 4	57.37
1.605	6	9 3 0	57.37
1.605	1	5 5 2	57.38
1.5981	1	-9 1 2	57.63
1.5904	3	1 5 3	57.94
1.5806	3	6 6 0	58.33
1.5806	1	10 0 0	58.33
1.5805	1	2 0 4	58.34
1.5764	1	-3 7 1	58.50
1.5697	3	8 2 2	58.78
1.5665	2	8 4 1	58.91
1.5665	2	4 4 3	58.91
1.5623	1	7 5 1	59.08
1.5561	1	6 2 3	59.34
1.5239	1	-7 3 3	60.73
1.5183	1	-4 2 4	60.97
1.5183	1	-8 4 2	60.98
1.5177	1	6 6 1	61.00
1.5168	3	3 1 4	61.04
1.5107	1	3 5 3	61.31
1.5054	1	-5 1 4	61.55
1.5052	1	-7 5 2	61.56
1.4933	3	-9 3 2	62.11
1.4932	2	-3 3 4	62.11
1.4928	1	5 7 0	62.13

Beryllium Calcium Iron Magnesium Aluminum Phosphate Hydroxide Hydrate, Roscherite, $Be_2Ca(Fe_{0.3}Mg_{0.7})_2Al_{0.67}(PO_4)_3(OH)_3\cdot 2H_2O$ - (continued)

d(A)	I	h	kl		2Θ(°) λ - 1.540598Å
1.4923	2	7	1	3	62.15
1.4912	2	-8	2	3	62.20
1.4807	1	9	1	2	62.70
1.4676	2	0	6	3	63.32
1.4643	3	-3	7	2	63.48
1.4594	1	-2	6	3	63.72
1.4571	2	-6	0	4	63.83
1.4568	2	-6	6	2	63.85
1.4422	1	5	7	1	64.57
1.4354	1	-10	2	2	64.91
1.4352	7	-2	4	4	64.92

. , 4 20 3,51 5,04 ,057	.10 .42	.127	1700 74 2		
Structure	Cal	culated I	Pattern (Pea	k heights)	
Triclinic, $C\overline{l}$ (2), $Z=2$. The structure was refined by Fanfani et al. [1977]. The material	d(A)	I	hkl	2Θ(°) λ - 1.54059	98Å
used in the structure determination was from					
Foote Mine, NC.	9.54	100	-1 1	0+ 9.26	
	7.94	11	2 0	0 11.14	
Atom positions	6.71	2	0 0	1 13.18	
The trivalent cations Fe, Mn and Al filled	5.981	90	0 2	0 14.80	
only $2/3$ of the special positions at 0, 0, $\frac{1}{2}$,	5.654	11	-1 -1		
the rest being void. All other atoms were in					
the 4 general positions of the C-centered	5.576	4	-1 1	1 15.88	
arrangement [ibid.]. The z coordinate for	5.342				
		6		1+ 16.58	
O(4B) was taken as + 0.1754 and the z coordi-	4.935	2		1 17.96	
nate for O(5A) was taken as + 0.9195.	4.839	40	3 1		
	4.507	3	0 -2	1 19.68	
Polymorphism					
A monoclinic roscherite exists and has a very	4.423	10	0 2	1 20.06	
similar atomic arrangement with partial dis-	4.008	5	-2 -2	1 22.16	
order of the trivalent cations over the sites	3.952	2	-2 2	1 22.48	
$(0, 0, 0)$ and $(0, 0, \frac{1}{2})$. Its chemical compo-	3.786	5	3 1		
sition is somewhat different, including the	3.404	8		1 26.16	
replacement of most of the manganese by	3.404	J	1 3	20.10	
	2 252	0.1	1 2	1+ 26.56	
magnesium [Fanfani et al., 1977].	3.353	21	-1 3		
* · · ·	3.307	6	4 2	0+ 26.94	
Lattice constants	3.229	8	-1 -1	2 27.60	
a = 15.922(5) Å	3.182	94	- 2 0		
b = 11.966(4)	3.140	20	1 -1	2 28.40	
c = 6.741(1)	3.110	18	1 1	2 28.68	
$\alpha = 91.07(8)^{\circ}$			- 5 1		
$\beta = 94.35(8)$	3.068	18	2 0		
$\gamma = 89.99(8)$	3.014	36		2 29.62	
•	2.992	11	0 4	0 29.84	
(published values: $a = 15.921(5) \text{ A}$,	2.951	5	0 -2	2+ 30.26	
$b = 11.965(4)$, $c = 6.741(1)$, $\alpha = 91^{\circ}4(5)'$,					
$\beta = 94^{\circ}21(5)', \ \gamma = 89^{\circ}59.5(5.0)'$ [Fanfani et al.,	2.906	5	0 2	2 30.74	
	2.864	9	-3 - 1	2 31.20	
1977]).	2.843	11	-3 1	2 31.44	
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2.831	9	-2 -2		
CD cell: $a = 9.959 \text{ A}, b = 9.957, c = 6.741$	2.798	48	2 4		
$\alpha = 92.83^{\circ}, \beta = 94.12, \gamma = 73.85, \text{ sp. gp. P1};$	2.750	40	2 7	31.70	
a/b = 1.0002, $c/b = 0.6770$	0 751	2	0 . 6	1 22 52	
	2.751	3		1 32.52	
Volume o	2.722	6	5 -1		
1280.4 Å ³	2./14	6	5 1	1+ 32.98	
	2.682	3	3 -1		
Density	2.645	43	6 0	0 33.86	
(calculated) 2.888 g/cm ³					
(Calculated) 2.888 g/Ciii	2.593	3	- 2 4	1 34.56	
m ,	2.585	3	-1 -3	2 34.68	
Thermal parameters	2.576	5	2 -4		
Isotropic [Fanfani et al., 1977]	2.536	6	1 -3		
	2.485	4	1 3		
Scattering factors	2.403	7	1 3	2, 30.12	
Zero ionization [International Tables, 1962]	0 /7/	,	/ 0	0 06 00	
	2.474	4		2 36.28	
Scale factors (integrated intensities)	2.448	2	-4 -2		
$y = 0.1244 \times 10^{-3}$	2.420	14	- 6 2		
	2.384	9	-3 - 3	2+ 37.70	
I/I _{corundum} (calculated) = 0.728 for	2.366	6	-1 5	0+ 38.00	
reflection with hkl = 020.					
	2.348	4	-3 3	2 38.30	
References	2.295	2	5 -3		
Fanfani, L., Zanazzi, P. F., and Zanzari, A. R.	2.274	4	-4 4		
	1		0 -4		
(1977). Tschermak's Mineral. Petrogr. Mitt.	2.253	11			
24, 169.	2.228	22	-1 5	1+ 40.46	
International Tables for X-ray Crystallography					
III (1962). (The Kynoch Press, Birmingham,					
Eng.) p. 202.	l				
100					

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roscherite, $Be_4Ca_2(Mn_{3.91}Mg_{.04}Ca_{.05})(Al_{.13}Fe_{.42}Mn_{.12})(PO_4)_6(OH)_4\cdot 6H_20 \text{ - (continued)}$

	Cal	culated	Pattern	(Pe	ak l	neights)
d(Å)		I		hkl		2Θ(°) λ - 1.540598Å
2.2 2.1 2.1 2.1 2.1	96 80 60	20 10 4 4 3	-1 -1 3 -6	-1 1 5 0 1	3+ 3+ 0+ 2+ 3	40.78 41.06 41.38 41.78 41.90
2.1 2.1 2.0 2.0 2.0	42 05 95 76	2 2 2 7 9	2 2 -3 -2 7	-4 4 -1	2 2+ 3 3	42.16 42.94 43.14 43.56 43.66
2.0 2.0 2.0 2.0 2.0	67 53 46 40	11 4 4 3 2	7 -2 3 -6 -6	1 2 5 -2 2	1+ 3 1+ 2 2	43.76 44.08 44.24 44.38 44.72
2.0 1.9 1.9 1.9	94 84 76	6 5 3 4 2	-4 0 8 -4 -1	-4 6 0 4 -5	2+ 0 0 2+ 2	45.20 45.44 45.68 45.88 46.24
1.9 1.9 1.9 1.9	33 29 09	3 8 7 2 2	5 5 -1 6 -4	-3 3 5 -2 2	2 2+ 2+ 2+ 3	46.42 46.96 47.08 47.60 47.76
1.8 1.8 1.8 1.8	83 71 67	2 1 1 2 1	6 8 -5 -5 -8	2 2 1 -5 -2	2 0+ 3 1+ 1+	47.90 48.30 48.62 48.74 49.18
1.8 1.8 1.7	18 08 89	2 2 3 4 6	5 3 5 3 -4	-5 -5 5 5 6	1 2 1+ 2+ 0+	49.96 50.14 50.42 51.02 51.22
1.7 1.7 1.7 1.7	69 60 57	5 7 5 5 5	0 -8 -6 -2 5	4 0 -4 4 -1	3+ 2 2 3 3	51.36 51.64 51.90 52.02 52.12
1.7 1.7 1.7 1.6 1.6	29 00 92	7 4 7 3 5	-6 0 0 -8 -4	4 -6 6 2 -4	2+ 2 2+ 2 3	52.50 52.92 53.88 54.16 54.40
1.6 1.6 1.6 1.6	76 54 40	10 8 15 4 4	0 6 -8 1 1	0 -4 4 1 7	4 2 0+ 4+ 1	54.58 54.72 55.52 56.04 56.12

d(Å)	Ι	hkℓ	2Θ(°) λ - 1.540598Å
1.633	4	1 -5 3+	56.30
1.627	3	-8 4 1+	56.52
1.622	2	-1 5 3	56.70

Calculated Pattern			(Integrated)			
d(A)	Ι		hkl		2Θ(°) λ - 1.540598A	
9.56		-1	1	0	9.24	
9.5		1	1	0	9.25	
7.94		2	0	0	11.14	
6.72		0	0	1	13.16	
5.98	32 100	0	2	0	14.80	
5.65	59 12	-1	-1	1	15.65	
5.5	79 3	- 1	1	1	15.87	
5.34	6 5	1	1	1	16.57	
5.33	32 1	-2	0	1	16.61	
4.94	7 1	2	0	1	17.91	
4.8	42 21	-3	1	0	18.31	
4.83		3	1	0	18.33	
4.78		-2	2	0	18.55	
4.7		2	2	0	18.57	
4.5		0	-2	1	19.67	
4.4	27 12	0	2	1	20.04	
4.04		-3	1	1	21.93	
4.00		-2	-2	1	22.16	
3.95		-2	2	1	22.47	
3.8		3	-1	1	23.28	
3.79	90 4	3	1	1	23.45	
3.78		2	2	1	23.48	
3.40		-1	-3	1	26.14	
3.3		0	0	2	26.50	
3.3		-1	3	1	26.56	
3.3	53 2	1	-3	1	26.57	
3.30		-4	2	0	26.92	
3.30		4	2	0	26.95	
3.23		-1	-1	2	27.58	
3.20		-1	1	2	27.85	
		2	2			
3.18		-3	3	0	27.98	
3.18		3	3	0	28.01	
3.18		-2	0	2	28.02	
3.14		1 1	-1 1	2	28.40 28.67	
3.0		- 5	1	0	29.06	
3.00		5	1	0	29.08	
3.0		2	0 4	2	29.62	
2.99		0	- 2	0	29.85 30.24	
2.9		. 2				
2.90		-3	-3 2	1 2	30.31	
		0 4	2		30.74	
2.8		-5	-1	1	30.99	
2.8		-3	-1 -1	1 2	31.06 31.19	
2.00	,,	-3	_ 1	2	31.19	

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roshcherite, Be $_4$ Ca $_2$ (Mn $_{3.91}$ Mg $_{.04}$ Ca $_{.05}$)(Al $_{.13}$ Fe $_{.42}$ Mn $_{.12}$)(PO $_4$) $_6$ (OH) $_4$ ·6H $_2$ O - (continued)

d(A)	I	hkl λ	20(°) - 1.540598A	d(A)	
2.844	12	-3 1 2	31.43	2.196	-
2.830	6	-2 -2 2	31.59	2.181	
2.812	1	3 3 1	31.80	2.179	
2.800	30	-2 4 0	31.94	2.161	
2.798	31	2 4 0	31.96	2.160	
2.790	3	-2 2 2	32.06	2.152	
2.752	2	0 -4 1	32.51	2.141	
2.723	6	5 -1 1	32.87	2.105	
2.712	3	5 1 1	33.00	2.095	
2.710	2	2 -2 2	33.03	2.085	
2.684	2	3 -1 2	33.36	2.077	
2.666	1	-4 0 2	33.59	2.072	
2.665	4	3 1 2	33.60	2.068	
2.646	55	6 0 0	33.85	2.067	
2.624	1	-2 -4 1	34.14	2.053	
2.593	3	-2 4 1	34.56	2.045	
2.584	1	-1 -3 2	34.69	2.044	
2.576	4	2 -4 1	34.80	2.039	
2.543	2	2 4 1	35.26	2.025	
2.537	2	-1 3 2	35.35	2.006	
2.537	4	1 -3 2	35.36	2.004	
2.492	3	1 3 2	36.02	1.994	
2.486	2	-5 3 0	36.11	1.985	
2.483	1	5 3 0	36.15	1.977	
2.474	3	4 0 2	36.29	1.970	
2.448	3	-4 -2 2	36.68	1.962	
2.423	2	-4 2 2	37.08	1.954	
2.421	9	-6 2 0	37.11	1.939	
2.419	8	6 2 0	37.14	1.938	
2.390	4	-4 4 0	37.60	1.934	
2.387	4	4 4 0	37.65	1.933	
2.384	5	-3 -3 2	37.70	1.932	
2.366	4	-1 5 0	37.99	1.928	
2.366	3	1 5 0	38.01	1.927	
2.349	4	-3 3 2	38.29	1.925	
2.298	1	4 -2 2	39.17	1.921	
2.296	1	5 -3 1	39.21	1.909	
2.294	1	-4 -4 1	39.24	1.902	
2.274	3	-4 4 1	39.60	1.895	
2.255	8	0 -4 2	39.95	1.872	
2.253	7	-1 -5 1	39.99	1.867	
2.230	1	4 -4 1	40.41	1.864	
2.229	9	-7 1 0	40.44	1.851	
2.228	8	7 1 0	40.46	1.824	
2.227	12	-1 5 1	40.47	1.818	
2.214	10	0 4 2	40.73	1.811	
2.211	16	-1 -1 3	40.78	1.808	
2.208	3	4 4 1	40.84	1.789	
2.200	1	-2 0 3	40.99	1.788	
2.198	2	-2 -4 2	41.02	1.783	

d(A)	I	hkl	2Θ(°) 。 λ - 1.540598A
2.196	8	-1 1 3	41.07
2.181	2	-3 5 0	41.36
2.179	2	3 5 0	41.40
2.161	1	-2 4 2	41.77
2.160	4	-6 0 2	41.79
2.152	2	1 1 3	41.95
2.141	2	2 -4 2	42.17
2.105	1	2 4 2	42.94
2.095	1	-3 -1 3	43.14
2.085	2	0 2 3	43.36
2.077	6	-2 -2 3	43.54
2.072	5	7 -1 1	43.65
2.068	2	-5 -3 2	43.74
2.067	8	7 1 1	43.76
2.053	4	-2 2 3	44.08
2.045 2.044 2.039 2.025 2.006	2 2 2 2 2 3	-5 3 2 3 5 1 -6 -2 2 -6 2 2 6 0 2	44.24 44.27 44.40 44.73 45.16
2.004	5	-4 -4 2	45.20
1.994	6	0 6 0	45.45
1.985	2	8 0 0	45.68
1.977	4	-4 4 2	45.87
1.970	1	-1 -3 3	46.04
1.962	2	-1 -5 2	46.23
1.954	3	5 -3 2	46.43
1.939	2	-1 3 3	46.82
1.938	2	1 -3 3	46.83
1.934	2	-2 6 0	46.93
1.933 1.932 1.928 1.927 1.925	3 4 2 1	2 6 0 5 3 2 -1 5 2 -7 -1 2 -6 4 1	46.96 46.99 47.09 47.12 47.17
1.921 1.909 1.902 1.895 1.872	1 1 2 1	-4 -2 3 6 -2 2 -4 2 3 6 2 2 -5 1 3	47.28 47.59 47.77 47.96 48.60
1.867	1	-5 -5 1	48.73
1.864	1	7 -3 1	48.81
1.851	1	-8 -2 1	49.19
1.824	2	5 -5 1	49.95
1.818	2	3 -5 2	50.14
1.811	2	4 -2 3	50.34
1.808	3	5 5 1	50.42
1.789	3	3 5 2	51.00
1.788	2	-2 -4 3	51.05
1.783	3	-4 6 0	51.20

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roshcherite, Be $_4$ Ca $_2$ (Mn $_{3.91}$ Mg $_{.04}$ Ca $_{.05}$)(Al $_{.13}$ Fe $_{.42}$ Mn $_{.12}$)(PO $_4$) $_6$ (OH) $_4$ ·6H $_2$ O - (continued)

d(A)	I	hkl	2Θ(°) λ - 1.540598Å
1.782	1	3 3 3	51.23
1.781	3	4 6 0	51.26
1.777	1	8 2 1	51.36
1.777	2	0 4 3	51.37
1.769	9	-8 0 2	51.64
1.760	5	-6 -4 2	51.90
1.757	3	-2 4 3	52.00
1.753	3	5 -1 3	52.12
1.745	1	- 9 1 0	52.38
1.745	1	5 1 3	52.38
1.745	1	9 1 0	52.40
1.742	5	-6 4 2	52.49
1.741	2	2 -4 3	52.51
1.729	6	0 -6 2	52.91
1.705	1	-5 -5 2	53.71
1 701	4	0 6 2	E2 94
1.701			53.86
1.700	3	-8 -2 2	53.89
1.700	1	-1 7 0	53.90
1.699	1	1 7 0	53.92
1.692	2	-8 2 2	54.17
1.685	4	-4 -4 3	54.40
1.680	12	0 0 4	54.58
1.676	3	6 -4 2	54.74
1.670	1	-2 0 4	54.95
1.660	2	-4 4 3	55.29
1.658	4	-1 -7 1	55.37
1.658	1	9 1 1	55.38
1.657	3	6 4 2	55.41
1.655	2	8 0 2	55.49
1.655	9	-8 4 0	55.49
1.653	8	8 4 0	55.56
1.645	2	-7 -1 3	55.84
1.644	3	-1 7 1	55.90
1.638	1	1 1 4	56.11
1.637	2	1 7 1	56.14
1.633	3	1 -5 3	56.30
1.627	1	-3 7 0	56.52
1.627	2	-8 4 1	56.53
1.621	1	-1 5 3	56.74
1,021		1 3 3	55.77

60.56

62.48

63.16

63.32

Structure	Calo	culated Pa	ttern ((Pea	k heig	ghts)
Monoclinic, P2/a (13), Z = 2. The structure was determined by Simonov et al. [1976], for material from the Solongo deposits in the Urals.	d(A)	I	ŀ	nkl	λ ·	20(°) °
orars.	7.76	100	0	1	0	11.40
Atom positions	6.64	38	0	0	1	13.32
Calcium atoms were in special positions (3/4,	5.046	12	0	1	1	17.56
O, z). All other atoms were in general	4.576	13	-1			19.38
positions [ibid.].	3.952	20	1	1	1	22.48
Lattice constants	3.877	6	0	2	0+	22.92
Simonov et al. [1976]	3.346	76	-1	2	1+	26.62
0	3.173	14	2	1	0	28.10
a = 8.006(2) A	3.056	4	0	1	2	29.20
b = 8.012(2)	2.855	7	-2	2	1+	31.30
c = 6.649(2)						
$\gamma = 104.21(2)^{\circ}$	2.754	1		1		32.48
0	2.589	2		3		34.62
CD cell: $a = 8.012 \text{ Å}, b = 6.649, c = 8.006,$	2.524	43		0		35.54
$\beta = 104.21^{\circ} \text{ sp. gp. } P2/c; a/b = 1.2050,$	2.468	35	- 3		1+	36.38
c/b = 1.2041	2.413	13	0	3	1	37.24
Volume o	2.295	23	2	1	2+	39.22
413.4 Å ³	2.216	2	0		3	40.68
113.7 11	2.167	7		3		41.64
Density	2.131	3		1		42.38
(calculated) 1.878 g/cm ³	2.092	1		1	3	43.22
	0.076	,			•	10.56
Thermal parameters	2.076	4	-3			43.56
Isotropic [Simonov et al., 1976]	2.042	1		3		44.32
	2.021	2		1		44.82
Scattering factors	1.971	16	-2			46.00
B ⁰ , Ca ⁰ , O ⁻ [Cromer and Mann, 1968]. H ⁰ [International Tables, 1962]	1.941	10	_		0	46.76
	1.936	12	-4			46.88
Scale factors (integrated intensities)	1.924	11	-2		_	47.20
$\gamma = 0.4656 \times 10^{-3}$	1.863	10		0		48.86
$I/I_{corundum}$ (calculated) = 1.05 for reflection	1.817	8		2	3+	50.16
with hkl = 010.	1.782	3	4	1	0	51.22
	1.776	8	-4	3	0	51.42
Additional pattern	1.722	3	4	1	1	53.16
1. PDF card 23-866 [Gode and Kuka, 1970]	1.716	3	-4	3	1	53.34
D. C	1.703	2	-1	3	3	53.80
References Cromer, D. T. and Mann, J. B. (1968). Acta	1.683	1	3	0	3+	54.48
Crystallogr. A24, 321.						
Gode, G. K. and Kuka, P. Ya. (1970). Russ. J.	1.678	3		2	2+	54.66
Inorg. Chem. 15, 603.	1.674	4		4	2+	54.80
International Tables for X-ray Crystallography	1.662	3		0	4	55.22
III (1962). (The Kynoch Press, Birmingham,	1.646	3	2	2	3	55.80
Eng.) p. 202.	1.625	2	0	1	4+	56.58
Simonov, M. A., Yamanova, N. A., Kazanskaya,	1.608	1	-1	1	4	57.26
E. V., Egorov - Tismenko, Yu. K., and	1.587	3	4	2	0	58.08
Belov, N. V. (1976). Sov. Phys. Dokl. 21,	1.571	1		1	2+	58.72
314.	1.553	4		5	0+	59.46
	1.544	2	2	4	1	59.86
	1 527	2	_ /.	/.	1	60.14
	1.537	2	-4 2	4	1 4+	60.14

2

1

1

1.528 1.4853

1.4709

1.4676

2

-4 1 3

1

0 4+

2 4+

-3 5 1

Calcium Borate Hydrate, Hexahydroborite, $Ca[B(0H)_4]_2 \cdot 2H_20$ - (continued)

d(Å)	I	hkl	2Θ(°) λ - 1.540598A
1.4618	2	2 3 3+	63.60
1.4325	1	2 4 2	65.06
1.4286	2	-2 5 2+	65.26
1.4094	1	-1 3 4	66.26

	culated	Pattern	(In	teg	rated)
d(A)	I		hkl		2Θ(°) ° λ - 1.540598Å
7.77	100	0	1	0	11.38
6.65	38	0	0	1	13.31
5.051	13	0	1	1	17.54
4.581	14	-1	1	1	19.36
3.955	21	1	1	1	22.46
3.883	3	0	2	0	22.88
3.881	2	2	0	0	22.90
3.872	3	-2	1	0	22.95
3.353	27	0	2	1	26.56
3.351	16	2	0	1	26.58
3.347	27	-1	2	1	26.61
3.346	24	-2	1	1	26.62
3.324	7	0	0	2	26.79
3.174	16	2	1	0	28.09
3.056	4	0	1	2	29.20
2.865	3	1	2	1	31.19
2.864	2	_ 2	1	1	31.20
2.854	6	-2	2	1	31.32
2.754	2	1	1	2	32.48
2.589	3	0	3	0	34.62
2.525	46	2	0	2	35.53
2.523	6	-1	2	2	35.55
2.469	19	-1	3	1	36.35
2.468	25	-3	1	1	36.37
2.460	1	2	2	0	36.50
2.449	2	-2	3	0	36.67
2.413	15	0	3	1	37.24
2.411	2	3	0	1	37.27
2.298	2	-2	3	1	39.17
2.297	2	-3	2	1	39.18
2.296	3	1	2	2	39.20
2.296	22	2	1	2	39.21
2.290	3	-2	2	2	39.30
2.216	2	0	ō	3	40.68
2.168	8	1	3	1	41.63
2.131	3	0	1	3	42.38
2.131	1	1	0	3	42.38
2.091	1	-1	1	3	43.22
2.076	5	- 3	1	3 2	43.56
2.043	1	0	3	2	44.31

d(A)	I	hkl	2Θ(°) 。 λ - 1.540598A
2.021	3	1 1 3	44.82
1.977	8	2 2 2	45.86
1.972	16	- 2 3 2	45.99
1.971	1	- 3 2 2	46.00
1.942	10	0 4 0	46.75
1.937	3	- 2 4 0	46.86
1.936	6	- 4 2 0	46.89
1.925	3	0 2 3	47.18
1.925	2	2 0 3	47.19
1.924	2	- 1 2 3	47.21
1.924	6	- 2 1 3	47.21
1.917	1	- 4 1 1	47.40
1.866	4	2 3 1	48.75
1.866	3	3 2 1	48.76
1.864	2	0 4 1	48.82
1.863	6	4 0 1	48.86
1.860	1	- 2 4 1	48.94
1.817	9	1 2 3	50.16
1.815	5	- 2 2 3	50.24
1.782	2	4 1 0	51.21
1.776	10	- 4 3 0	51.41
1.722	3	4 1 1	53.16
1.716	2	- 4 3 1	53.35
1.703	3	- 1 3 3	53.80
1.683	1	3 0 3	54.47
1.678	2	3 2 2	54.65
1.674	4	-2 4 2	54.80
1.662	4	0 0 4	55.21
1.646	4	2 2 3	55.79
1.625	2	0 1 4	56.58
1.608	1	-1 1 4	57.26
1.587	4	4 2 0	58.08
1.571	1	4 1 2	58.73
1.555	2	- 5 1 1	59.39
1.553	4	0 5 0	59.46
1.544	3	2 4 1	59.85
1.537	1	-4 4 1	60.14
1.4854	1	-4 1 3	62.47
1.4726	1	1 2 4	63.08
1.4676	1	-3 5 1	63.32
1.4617	2	2 3 3	63.60
1.4326	1	2 4 2 -2 5 2	65.06
1.4288	1		65.25
1.4271	1	-4 4 2	65.34
1.4096	1	- 1 3 4	66.25

 $\begin{array}{c} \text{Calcium Chromium Iron Titanium Oxide, Loveringite,} \\ \text{Ca.}_{72}\text{RE.}_{33}(\text{Y},\text{Th,U,Pb})._{05}\text{Ti}_{12.48}\text{Fe}_{3.38}\text{Cr}_{2.24}\text{Mg.}_{92}\text{Zr.}_{58}\text{Al.}_{39}\text{V.}_{21}\text{Mn.}_{04}\text{O}_{38} \end{array}$

Structure

Hexagonal, $R\bar{3}$ (148), Z=3, isostructural with senaite. The structure was refined by Gatehouse et al. [1978] using rhombohedral positions. Those were used to calculate the powder pattern which was transformed to the hexagonal setting given here. The sample used for the structure work came from the Jimberlana Intrusion near Norseman, Western Australia.

Atom positions

M(0) in 1(a) .72 calcium +.23 RE (as .1284 lanthanum and .1016 cerium) +.017 lead +.014 yttrium +.011 uranium +.006 thorium

M(1) in 1(b) .58 zirconium +.32 magnesium +.1 RE
(as .0285 hafnium, .0259 cerium,
.0245 neodymium and .0236 holmium)

M(2) in 2(c) partially vacant, with 1.23 iron and 0.6 magnesium

M(3) in 6(f) partially vacant, with 2.24 chromium +2.19 iron +.86 titanium +.21 vanadium

M(4) in 6(f) 5.81 titanium and .19 aluminum

M(5) in 6(f) 5.81 titanium and .19 aluminum 6(f) 6 oxygen in each of 6 different sites

2(c) 2 oxygen

Electron microprobe analysis results gave weight percents of the elements as oxides, and the unit cell composition was normalized to 38 oxygen. Distribution of the cations in sites M(0) to M(5) inclusive was guided by the results for senaite and crichtonite which showed ordering sequences based on the size of the cations [Gatehouse et al., 1978]. The Mn was combined with the Fe in sites M(2) and M(3).

Lattice constants

a = 10.337 Å c = 20.676

c/a = 2.0002

(published values: $a = 9.117(4) \stackrel{\circ}{A}$, $\alpha = 69.07(1)^{\circ}$ [Gatehouse et al., 1978])

Volume o 1913.4 A³

Density

(calculated) 4.415 g/cm³

Thermal parameters

Isotropic [Gatehouse et al., 1978]

Scattering factors
A1³⁺, Ce⁴⁺, Cr³⁺, Fe³⁺, Hf⁴⁺, Ho³⁺, La³⁺,
Mg²⁺, Nd³⁺, O¹⁻, Pb²⁺, Th⁴⁺, Ti⁴⁺, U⁴⁺,
V⁵⁺, Y³⁺, Zr⁴⁺ [International Tables, 1974]
Ca²⁺ [Cromer and Mann, 1968]

Ca²⁺ [Cromer and Mann, 1968] The factors for cerium, lanthanum and zirconium were corrected for dispersion [Cromer and Liberman, 1970] Scale factors (integrated intensities) $\gamma = 0.06676 \times 10^{-3}$ I/I corundum = 0.624, for reflection with hexagonal hkl = 024.

References

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Phys. 53, 1891.

Gatehouse, B. M., Grey, I. E., Campbell, I. H., and Kelly, P. (1978). Amer. Mineral. 63, 28.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 99.

	culated	Pattern	(Pe	ak hei	ghts)
d(Å)	I		hkl	λ	2Θ(°) 。 - 1.540598A
6.89	1	0	0	3	12.84
5.16	1	1	1	0	17.16
4.476	9	1	0	4	19.82
4.371	3	0	2	1	20.30
4.134	23	1	1	-3+	21.48
3.751	13	0	1	5	23.70
3.443	3	0	0	6	25.86
3.383	75	0	2	4	26.32
3.339	7	2	1	1	26.68
3.216	5	1	2	2	27.72
3.038	71	2	0	5	29.38
2.984	31	3	0	0	29.92
2.866	100	1	1	-6+	31.18
2.831	72	1	2	-4+	31.58
2.807	12	1	0	7	31.86
2.738	31	0	3	3+	32.68
2.618	40	1	2	5+	34.22
2.585	9	2	2	0	34.68
2.465	53	3	1	-1	36.42
2.414	28	3	1	2+	37.22
2.297	2	0	0	9	39.18
2.238	57	3	1	-4+	40.26
2.128	59	3	1	5+	42.44
2.099	5	1	1	-9+	43.06
2.054	3	1	2	8+	44.06
2.015	4	1	0	10+	44.96
1.968	1	0	4	5	46.08
1.954	7	1	4	0+	46.44
1.909	12	2	3	-4	47.60
1.901	16	3	1	- 7	47.82
1.878	6	0	2	10+	48.42
1.839	17	2	3	5	49.52
1.791	50	3	1	8	50.96
1.764	10	2	1	10	51.78
1.723	4	0	0	12	53.12

d(A)	I	hkl	2Θ(°)
		λ -	1.540598A
1.700	25	1 4 6+	53.90
1.686	8	2 4 1+	54.36
1.643	11	5 0 5	55.92
1.635	4	1 1 -12+	56.22
1.608	10	4 2 -4+	57.26
1.589	61	3 1 -10	58.00
1.566	9	4 2 5+	58.94
1.541	10	3 3 -6+	59.98
1.535	9	5 1 4+	60.22
	2		
1.519	2	4 0 10	60.96
1.4987	28	3 1 11+	61.86
1.4883	3	4 1 9+	62.34
1.4717	1	5 0 8	63.12
1.4680	2	2 4 7+	63.30
1.4573	6	6 0 3+	63.82
1.4392	8	2 1 13+	64.72
1.4336	61	2 5 0	65.00
1.4155	6	4 3 4	65.94
1.4030	7	2 0 14+	66.60
1.3865	6	4 3 -5+	67.50
1.3782	2	3 3 -9+	67.96
1.3690	10	0 6 6+	68.48
1.3535	5	1 2 14+	69.38
1.3393	6	3 1 -13+	70.22
1.3317	5	1 1 -15	70.68
1.3236	2	5 2 -6+	71.18
1.3200	2	6 1 -4	71.40
1.3172	2	3 4 -7+	71.58
1.3093	2	2 4 10	72.08
	2		
1.2962	2	6 1 5+	72.92
1.2923	3	1 4 12+	73.18
1.2694	2	1 3 -14+	74.72
1.2574	1	2 4 -11+	75.56
1.2515	1	3 0 15+	75.98
1.2415	3	0 2 16+	76.70
1.2390	6	6 2 1	76.88
1.2325	2	6 2 -2	77.36
1.2216	3	0 7 5+	78.18
1.2185	3	3 3 -12+	78.42
1.2162	5	2 5 -9+	78.60
1 0007	2	, , , , ,	70.10
1.2097	3	4 4 6+	79.10
1.2072	6	1 2 -16+	79.30
1.1991	4	2 3 14+	79.94
1.1890	2	6 2 - 5	80.76
1.1861	2	7 1 0	01 00
1.1001	2	7 1 0	81.00

C	alculated	Pattern	(Int	tegra	ted)
d(Å)	I		hkl	λ	20(°) - 1.540598A
6.80	1	0	0	3	12.83
5.17	1	1	1	0	17.14
4.476	11	1	0	4	19.82
4.375	3	0	2	1	20.28
4.135	11	1	1	3	21.47
4.135 4.108 3.754 3.446 3.384	16 9 16 2 100	1 2 0 0	1 0 1 0 2	-3 2 5 6 4	21.47 21.62 23.68 25.83 26.32
3.339	6	2	1	1	26.67
3.216	6	1	2	2	27.72
3.037	97	2	0	5	29.38
2.984	40	3	0	0	29.92
2.867	56	1	1	6	31.17
2.867	80	1	1	-6	31.17
2.831	16	2	1	4	31.58
2.831	80	1	2	-4	31.58
2.805	8	1	0	7	31.88
2.738	22	3	0	3	32.68
2.738	20	0	3	3	32.68
2.619	47	1	2	5	34.21
2.619	10	2	1	-5	34.21
2.584	12	2	2	0	34.68
2.465	1	0	2	7	36.41
2.465 2.465 2.420 2.420 2.414	3 72 12 11 23	1 3 2 2 2 3	3 1 2 2 1	1 -1 3 -3 2	36.42 36.42 37.12 37.12 37.21
2.297	2	0	0	9	39.18
2.238		1	3	4	40.26
2.238		3	1	-4	40.26
2.225		2	1	7	40.51
2.225		1	2	-7	40.51
2.129		3	1	5	42.43
2.129		1	3	-5	42.43
2.099		1	1	9	43.05
2.099		1	1	-9	43.05
2.054		1	2	8	44.05
2.054 2.015 2.014 1.968 1.954	3 2 1	2 1 2 0 1		-8 10 2 5 0	44.05 44.96 44.96 46.08 46.45
1.954 1.909 1.909 1.901 1.879	1 16 . 20	4 3 2 3 1	3	0 4 -4 -7 3	46.45 47.61 47.61 47.82 48.39

d(A)	I	hkl 2Θ(°) ° λ - 1.540598A
1.879	3	4 1 3 48.39
1.879	2	4 1 -3 48.39
1.877	5	0 2 10 48.46
1.840	1	0 1 11 49.51
1.839	25	2 3 5 49.51
1.791	1	1 3 -8 50.96
1.791	76	3 1 8 50.96
1.784	1	4 0 7 51.17
1.784	1	5 0 -1 51.17
1.764	1	2 1 10 51.77
1.723	5	0 0 12 53.11
1.699	3	4 1 6 53.91
1.699	18	1 4 6 53.91
1.699	17	1 4 -6 53.91
1.699	1	4 1 -6 53.91
1.692 1.686 1.686 1.686 1.643	7 2 1 4	0 5 4 54.17 2 3 -7 54.36 3 2 7 54.36 2 4 1 54.37 1 2 11 55.91
1.643 1.635 1.635 1.608	17 2 2 1 5	5 0 5 55.92 1 1 12 56.23 1 1 -12 56.23 3 2 -8 57.25 2 4 4 57.25
1.608 1.603 1.589 1.589	8 1 1 95 1	4 2 -4 57.25 1 5 -1 57.44 1 3 10 58.00 3 1 -10 58.00 5 1 -2 58.00
1.566	2	1 0 13 58.93
1.566	7	4 2 5 58.94
1.566	5	2 4 -5 58.94
1.541	6	3 3 6 59.98
1.541	9	3 3 -6 59.98
1.535	3	1 5 -4 60.23
1.535	8	5 1 4 60.23
1.519	3	4 0 10 60.96
1.4986	39	3 1 11 61.86
1.4986	2	1 5 5 61.86
1.4986	3	5 1 -5 61.86
1.4920	1	6 0 0 62.17
1.4882	1	4 1 9 62.34
1.4718	1	5 0 8 63.12
1.4680	2	2 4 7 63.30
1.4582	4	6 0 3 63.77
1.4571	2	3 2 10 63.83
1.4571	1	2 3 -10 63.83
1.4570	4	4 3 -2 63.83
1.4394	4	1 2 -13 64.71

d(A)	I	hkl λ -	20(°) ° 1.540598A
1.4394	4	2 1 13	64.71
1.4335	96	2 5 0	65.01
1.4335	5	5 2 0	65.01
1.4155	8	4 3 4	65.94
1.4122	1	1 5 -7	66.11
1.4035 1.4035 1.4025 1.3865 1.3865	3 3 6 1 7	5 2 -3 5 2 3 2 0 14 3 4 5 4 3 -5	66.58 66.58 66.63 67.50
1.3783	1	3 3 -9	67.95
1.3692	9	6 0 6	68.47
1.3692	7	0 6 6	68.47
1.3536	4	2 1 -14	69.37
1.3536	3	1 2 14	69.37
1.3393 1.3393 1.3319 1.3319 1.3235	7 2 7 1	1 3 13 3 1 -13 1 1 15 1 1 -15 5 2 -6	70.22 70.22 70.67 70.67 71.18
1.3199	1	6 1 -4	71.41
1.3173	1	4 3 7	71.57
1.3173	1	3 4 -7	71.57
1.3093	2	2 4 10	72.07
1.2965	1	4 0 13	72.91
1.2964	1	6 1 5	72.91
1.2922	2	1 4 12	73.18
1.2922	2	2 4 -12	73.18
1.2693	1	3 1 14	74.73
1.2693	1	1 3 -14	74.73
1.2693	1	1 5 -10	74.73
1.2514	1	3 0 15	75.99
1.2514	1	0 3 15	75.99
1.2416	2	0 2 16	76.69
1.2414	2	7 0 4	76.70
1.2392 1.2326 1.2218 1.2162 1.2162	7 2 5 1	6 2 1 6 2 -2 0 7 5 5 2 9 2 5 -9	76.87 77.36 78.17 78.60 78.60
1.2162	2	2 5 9	78.60
1.2162	2	5 2 -9	78.60
1.2099	2	4 4 6	79.09
1.2099	3	4 4 -6	79.09
1.2072	5	1 2 -16	79.30
1.2071	3	6 2 4	79.31
1.1990	3	2 3 14	79.95
1.1990	1	3 4 -10	79.95
1.1990	1	4 3 10	79.95
1.1890	4	6 2 -5	80.76

Structure
Monoclinic, Cc (9), Z = 4. The structure
was determined by Sakae et al. [1978].

Atom positions
4(a) 2 phosphorus(1) and 2 sulfur(1)
4(a) 2 phosphorus(2) and 2 sulfur(2)

Four hydrogen atoms were not located in the structure determination. All other atoms are in general positions 4(a) and the "x" and "z" parameters were given to only 3 significant figures [ibid.].

Lattice constants

a = 5.721(5) A b = 30.994(5) c = 6.250(4) β = 117.26(6)°

(published values: a = 5.721(5) Å, b = 30.992(5), c = 6.250(4), $\beta = 117.26(6)$ ° [Sakae et al., 1978]).

CD cell: a = 6.248(4) Å, b = 30.994(5), $c = 5.721(5), \beta = 117.22(6)^{\circ}, \text{ sp. gp. Aa}(9);$ a/b = 0.2016, c/b = 0.1846.

Volume 985.15 A³

Density (calculated) 2.321 g/cm³

Thermal parameters
Isotropic [Sakae et al., 1978]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factor (integrated intensities) $\gamma = 0.3683 \times 10^{-3}$

References

International Tables for X-ray Crystallography
III (1962). (The Kynoch Press, Birmingham,
Eng.) p. 202.

Sakae, T., Nagate, H., and Sudo, T. (1978). Amer.
Mineral. 63, 520.

Calo	culated	Pattern	(Pea	k l	heights)
d(Å)	Ι		hkl		2Θ(°) λ - 1.540598Å
7.74 5.02 4.56 3.931 3.874	100 5 40 50 15	0 -1 1 -1 0	4 1 3 5 8	0 1+ 0+ 1+ 0	11.42 17.66 19.44 22.60 22.94
3.783 3.339 3.093 2.976 2.852	1 45 10 15 35	0 1 -1 -1	6 7 1 3 9	1 0+ 2+ 2+ 1+	23.50 26.68 28.84 30.00 31.34
2.812 2.779 2.733 2.707 2.615	10 15 15 1 5	-2 1 0 0	2 5 2 10 4	1 1+ 2 1 2	31.80 32.18 32.74 33.06 34.26
2.543 2.509 2.447 2.416 2.308	15 5 20 5 5	2 2 0 -2 -1	0 2 6 4 9	0+ 0+ 2 2+ 2+	35.26 35.76 36.70 37.18 39.00
2.282 2.158 2.126 2.102 2.088	5 1 5 10 5	2 -1 2 -2 -1	6 13 8 10 11	0+ 1+ 0+ 1 2+	39.46 41.82 42.48 43.00 43.30
2.068 2.031 1.976 1.966 1.936	5 5 5 10 1	0 -1 -2 -2 0	10 3 2 10 16	2+ 3+ 3+ 2+ 0	43.74 44.58 45.88 46.14 46.88
1.930 1.892 1.876 1.849 1.829	5 5 5 1 1	2 0 1 -3 0	4 12 7 3 16	1+ 2+ 2+ 2+ 1	47.04 48.06 48.48 49.24 49.82
1.812 1.798 1.775 1.731 1.716	15 5 5 10 5	-2 -3 1 0 -1	12 5 9 14 17	2+ 1+ 2+ 2+ 1+	50.72 51.44 52.86
1.669 1.650 1.646 1.635 1.583	5 1 1 1 1	-1 -3 0 -3	11 9 18 5 7	3+ 1+ 1 3+ 3+	55.66 55.82 56.20
1.573 1.564 1.554 1.547 1.541	1 1 1 5	-1 -1 -2 -2 -2	0 2	2+ 3+ 4+ 4+ 2+	59.02 59.44 59.74

Calcium Hydrogen Phosphate Sulfate Hydrate, $Ca_2HPO_4SO_4\cdot 4H_2O$ - (continued)

	Calculated	Pattern (In	ntegrated)
d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
7.75 5.02 5.02 4.56 4.56	100 1 1 20 20	0 4 0 -1 1 1 1 1 0 -1 3 1 1 3 0	17.65 17.66 19.43
4.52 3.932 3.932 3.874 3.783	1 30 30 15 1	0 4 1 -1 5 1 1 5 0 0 8 0 0 6 1	22.59 22.60 22.94
3.340 3.339 3.094 3.093 2.978	25 25 5 5	-1 7 1 1 7 0 -1 1 2 1 1 1 -1 3 2	26.67 2 28.83 1 28.84
2.977 2.852 2.852 2.813 2.780	10 20 20 10 10	1 3 1 -1 9 1 1 9 0 -2 2 1 -1 5 2	1 31.34 31.34 1 31.79
2.779 2.734 2.707 2.615 2.545	10 15 1 10 5	1 5 1 0 2 2 0 10 1 0 4 2 -1 7 2	2 32.72 1 33.07 2 34.26
2.544 2.544 2.543 2.510 2.509	5 5 5 5 5	1 7 1 -2 0 2 2 0 0 -2 2 2 2 2 0	2 35.26 35.27 2 35.74
2.502 2.447 2.417 2.416 2.308	1 25 1 1 5	-2 6 1 0 6 2 -2 4 2 2 4 0 -1 9 2	2 36.70 2 37.17 37.18
2.308 2.282 2.281 2.159 2.159	5 1 5 1	1 9 1 -2 6 2 2 6 0 -1 13 1 1 13 0	2 39.46 39.47 1 41.81
2.126 2.126 2.102 2.088 2.088	5 5 10 1	-1 11 2	42.49 42.99
2.069 2.031 2.031 1.977 1.976	5 5 5 1 1	-1 3 3 1 3 2 -2 2 3	2 43.72 3 44.57 2 44.58 3 45.86 1 45.88

.0.			
d(Å)	I	hkl	2θ(°) 。
			λ - 1.540598A
1.966	5	-2 10 2	46.13
1.966	5	2 10 0	46.14
1.965	1	-1 5 3	46.16
1.964	1	1 5 2	46.17
1.937	1	0 16 0	46.86
1.930	5	-2 4 3	47.04
1.930	5	2 4 1	47.05
1.892	5	0 12 2	48.06
1.877	1	-1 7 3	48.47
1.876	1	-3 1 2	48.48
1.876	5	1 7 2	48.48
1.876	1	-3 1 1	48.49
1.829	1	0 16 1	49.81
1.812	10	- 2 12 2	50.31
1.812	10	2 12 0	50.31
1.799	5	-3 5 2	50.71
1.799	5	- 3 5 1	50.72
1.775	5	- 1 9 3	51.43
1.775	5	1 9 2	51.44
1.731	5	0 14 2	52.84
1.730	1	-3 7 2	52.87
1.730	1	- 3 7 1	52.88
1.716	1	-1 17 1	53.34
1.716	1	1 17 0	53.34
1.670	1	-2 14 2	54.94
1.670	1	2 14 0	54.95
1.669	1	-1 11 3	54.97
1.669	1	1 11 2	54.98
1.650	1	- 3 9 2	55.66
1.650	1	-3 9 1	55.67
1.645	1	0 18 1	55.85
1.584	1	-3 7 3	58.21
1.573	1	-1 17 2	58.65
1.573	1	1 17 1	58.66
1.547	5	-2 2 4	59.72
1.547	1	2 2 2	59.75
1.541	î	-2 16 2	59.98
1.541	ī	2 16 0	59.99

Cannabidio
Synonym 1. (1R-trans)-2-[3-Methyl-6-(1-methylethenyl)- 2-cyclohexen-1-yl]-5-pentyl-1,3-benezenediol
CAS registry no. 13956-29-1
Structure Monoclinic, $P2_1$ (4), $Z = 4$. The structure was refined by Jones et al. [1977].
Atom positions All atoms were in general positions 2(a). Sixty-eight hydrogen positions were not located.
Lattice constants a = 10.618(4) Å b = 10.650(5) c = 17.267(6) β = 95.30(4)°
(published values: $a = 10.617(4) \stackrel{\circ}{A}$, $b = 10.649(5)$, $c = 17.266(6)$, $\beta = 95.30(4)^{\circ}$ [Jones et al., 1977])
CD cell: $a = 17.267(6)$ Å, $b = 10.650(5)$, $c = 10.618(4)$, $\beta = 95.30(4)^{\circ}$; sp. gp. P2 ₁ ; $a/b = 1.6213$; $c/b = 0.9970$
Volume o 1944.2 A ³
Density (calculated) 1.074 g/cm ³ [Jones et al., 1977]
Thermal parameters Isotropic. For hydrogen atoms, overall B = 0.125. For other atoms, B, were estimated from U, for individual atoms.
Scattering factors Zero ionization [International Tables, 1962]
Scale factors (integrated intensities) $ \gamma = 2.067 \times 10^{-3} $ I/I (calculated) = 0.668 for reflections with hk ℓ = 011.
References International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Jones, P. G., Falvello, L., Kennard, O., Sheldrick, G. M., and Mechoulam, R. (1977). Acta. Crystallogr. <u>B33</u> , 3211.

	culated	Pattern	(Pe	ak he	eights)
d(A)	I		hkl	7	2Θ(°) • 1.540598A
17.18 10.57 9.40 9.05 8.60	4 5 32 100 33	0 1 -1 0 0	0 0 0 1	1 0 1 1 2	5.14 8.36 9.40 9.76 10.28
7.494	33	1	1	0	11.80
7.042	19	-1	1	1	12.56
6.702	30	1	1	1+	13.20
6.384	20	1	0	2	13.86
5.840	20	-1	1	2	15.16
5.727 5.474 5.323 5.187 5.081	4 3 5 6 34	0 1 0 -2 0	0 1 2 0 2	3 2 0 1	15.46 16.18 16.64 17.08
4.924	10	2	0	1	18.00
4.701	28	-1	1	3+	18.86
4.662	22	-2	1	1	19.02
4.530	11	1	2	1+	19.58
4.471	5	2	1	1	19.84
4.296	20	-2	1	2+	20.66
4.235	10	-1	2	2	20.96
4.085	23	1	2	2	21.74
4.005	24	2	1	2	22.18
3.987	26	0	1	4	22.28
3.901	15	0	2	3	22.78
3.860	3	1	0	4	23.02
3.841	3	-1	1	4	23.14
3.808	2	-2	1	3	23.34
3.736	7	-1	2	3+	23.80
3.717	8	2	0	3+	23.92
3.628	7	1	1	4	24.52
3.587	4	1	2	3	24.80
3.498	6	-2	0	4+	25.44
3.477	4	0	3	1	25.60
3.388	1	3	0	1	26.28
3.358	3	2	2	2+	26.52
3.341	3	-3	1	1+	26.66
3.321	3	-2	1	4+	26.82
3.283	3	1	3	1	27.14
3.257	2	-1	1	4	27.36
3.232	4	3		1+	27.58
3.213	5	-3		2+	27.74
3.160	2	3		2+	28.22
3.123	2	1		4	28.56
3.102 3.052 3.010 2.923 2.897	4 7 1 1	1 2 -3 -2 -2	2	2 4+ 3+ 4+ 5	28.76 29.24 29.66 30.56 30.84

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
2.859	3		31.26
2.735	2	1 2 5	32.72
2.717	1	3 2 2	32.94
2.677	2	2 1 5	+ 33.44
2.662	1	0 4 0	33.64
2.621	3	1 1 6	5+ 34.18
2.593	2	- 4 0 2	34.56
2.582	3	1 4 0)+ 34.72
2.562	2	-1 4 1	.+ 35.00
2.535	3	3 1 4	+ 35.38
2.499	1	- 3 3 1	.+ 35.90
2.452	1		+ 36.62
2.445	1	-3 3 2	2+ 36.72
2.424	1		37.06
2.410	1		37.28
2.373	1	-1 4 3	37.88
2.349	1		38.28
2.277	1		39.54
2.235	1	_	3+ 40.32
2.219	1	-1 2 7	
2.214	2	-1 3 6	6 40.72
2.147	1		7+ 42.06
2.119	1		7+ 42.64
2.088	î		5+ 43.30
2.004	i		5+ 45.22
1.997	1	0 5 3	3+ 45.38
1.971	1		1+ 46.00
1.936	1		7+ 46.88
1.748	1		2+ 52.28

	culated P		(111		14004)
d(A)	I		hkl		2Θ(°) ο λ - 1.540598A
17.19	3	0	0	1	5.14
10.57	5	1	0	0	8.36
9.40	29	-1	0	1	9.40
9.05	100	0	1	1	9.76
8.66	4	1	0	1	10.21
8.60	30	0	0	2	10.28
7.503	34	1	1	0	11.79
7.048	19	-1	1	1	12.55
6.717	21	1	1	1	13.17
6.689	14	0	1	2	13.23
6.387	20	1	0	2	13.85
5.846	20	-1	1	2	15.14
5.731	3	0	0	3	15.45
5.478	3 5	1	1	2	16.17
5.325	5	0	2	0	16.63

d(A)	I	hkl	2Θ(°) λ - 1.540598Å
5.189	5	-2 0 1	17.07
5.087	35	0 2 1	17.42
5.047	4	0 1 3	17.56
4.927	10	2 0 1	17.99
4.735	4	2 1 0	18.72
4.706	14	-1 1 3	18.84
4.701	13	-2 0 2	18.86
4.665	18	-2 1 1	19.01
4.633	6	-1 2 1	19.14
4.536	8	1 2 1	19.56
4.527	3	0 2 2	19.59
4.471	5	2 1 1	19.84
4.328	1	2 0 2	20.50
4.301	14	-2 1 2	20.64
4.298	7	0 0 4	20.65
4.237	10	-1 2 2	20.95
4.090	21	1 2 2	21.71
4.078	6	-2 0 3	21.78
4.010	22	2 1 2	22.15
3.986	23	0 1 4	22.29
3.901	16	0 2 3	22.78
3.859	2	1 0 4	23.03
3.840	2	-1 1 4	23.15
3.808	1	-2 1 3	23.34
3.752	3	2 2 0	23.70
3.737	5	-1 2 3	23.79
3.718	5	2 0 3	23.91
3.716	2	-2 2 1	23.92
3.628	7	1 1 4	24.51
3.616	1	2 2 1	24.60
3.587	3	1 2 3	24.80
3.524	2	-2 2 2	25.25
3.511	3	2 1 3	25.35
3.497	4	-2 0 4	25.45
3.477	3	0 3 1	25.60
3.391 `.363 3.359 3.345 3.340	1 1 2 1	3 0 1 -1 0 5 2 2 2 0 2 4 -3 1 1	26.26 26.49 26.52 26.63 26.67
3.322	2	-2 1 4	26.81
3.285	2	1 3 1	27.13
3.257	1	-1 2 4	27.36
3.238	2	-2 2 3	27.53
3.231	2	3 1 1	27.58
3.215	4	-3 1 2	27.73
3.207	2	-1 1 5	27.80
3.194	1	2 0 4	27.91
3.160	1	3 0 2	28.22
3.125	2	1 2 4	28.54

Cannabidiol, $C_{21}H_{30}O_2$ - (continued)

0			
d(A)	I	hkl	2Θ(°) 。
			λ - 1.540598Å
3.103	4	1 3 2	28.75
3.059	6	2 1 4	
3.051	3	1 1 5	29.25
3.049	1	2 2 3	
3.029	1	3 1 2	
2.923	1	-2 2 4	30.56
2.899	1	-2 1 5	
2.865	2	1 3 3	
2.860	2	3 2 1	
2.858	1	-3 0 4	
2.030	1	-3 0 4	31.27
2.849	1	-3 2 2	
2.733	1	1 2 5	32.74
2.718	1	3 2 2	32.93
2.679	2	2 1 5	33.42
2.662	1	0 4 0	33.63
2.631	1	0 4 1	34.05
2.623	1	-2 0 6	
2.620	1	1 1 6	
2.613	î	1 3 4	
2.595	2	-4 0 2	
2.333	2	4 0 2	. 54.54
2.582	3	1 4 0	34.72
2.562	2	-1 4 1	. 35.00
2.537	1	3 2 3	35.35
2.535	2	3 1 4	35.38
2.445	1	- 3 3 2	36.73
2.424	1	-4 1 3	37.06
2.411	1	1 2 6	
2.374	1	-1 4 3	
2.277	1	-3 1 6	
2.220	1	-1 2 7	
2.223		/	10.00
2.214	1	-1 3 6	
2.120	1	-2 2 7	42.62

Synonyms 1. L-3-Tropanylbenzoate-2-carboxylic acid	Calc	culated Pa	ttern	(Pe	ak he:	ights)
methyl ester hydrochloride 2. Cocaine muriate	d(Å)	I		hkl		20(°) - 1.540598A
CAS registry no.	10.72	100	0	0	2	8.24
53-21-4	9.28	53	Ö	1		9.52
55 1	7.43	20		1		11.90
Structure	7.19	30	_	Ō	_	12.30
Orthorhombic, P2 ₁ 2 ₁ 2 ₁ (19), Z = 4. The structure was refined by Gabe and Barnes	6.206	3		0		14.26
[1963].	6.129	8 '	1	1	0	14.44
[2500].	5.878	83		1		15.06
Atom positions	5.323	35		1		16.64
All atoms were in general positions 4(a). A	5.218	8		0		16.98
position was not located for the hydrogen associated with the chlorine in the hydro-	5.145	24		2		17.22
chloride.	5.007	9	0	2	1	17.70
	4.756	64		1		18.64
Lattice constants	4.648	55	1	1	3+	19.08
0	4.388	25	1		-	20.22
a = 7.633(1) A $b = 10.301(1)$	4.267	32	1	2	0	20.80
c = 21.460(3)	4.184	20	1	2	1	21.22
0	4.037	21	1	1	4	22.00
(published values: a = 7.633(1) A,	3.966	32	1	2	2	22.40
b = 10.300(1), c = 21.459(3) [Gabe and	3.815	3		0		23.30
Barnes, 1963])	3.739	6	1			23.78
CD cell: $a = 10.301(1) A$, $b = 21.460(3)$,	3.714	5	0	2	4	23.94
$c = 7.633(1)$; sp. gp. $P2_12_12_1$; $a/b = 0.4800$,	3.666	10	_	2		24.26
c/b = 0.3557.	3.579	38		1		24.86
	3.515	38		1		25.32
Volume 0 1687.3 A ³	3.394	18	2			26.24
	3.339	17	1	2	4	26.68
Density	3.297	3	_	2		27.02
(calculated) 1.338 g/cm ³	3.269	6		3		27.26
(measured) 1.342 g/cm ³ [Gabe and Barnes, 1963]	3.239	15		0		27.52
	3.200	5		1		27.86
Thermal parameters			_	_	_	
Isotropic [Gabe and Barnes, 1963]	3.129	13	1	3	0	28.50
	3.089	41	1	1		28.88
Scattering factors	3.066	17	2	2	0	29.10
Cl^{-} , C^{0} , H^{0} , N^{0} , O^{0} [International Tables,	3.028	15	1			29.48
1962]	3.006	13	1	3	2	29.70
Scale factors (integrated intensities)	2.976	12	2	1	4	30.00
$\gamma = 0.4587 \times 10^{-3}$	2.976	14	2			30.30
$I/I_{corundum}$ (calculated) = 0.470 for reflection	2.868	14	1			31.16
		5	2		3	31.72
with $hk\ell = 002$.	2.819 2.741	9	1		5 6+	32.64
Additional patterns	2.741	7		2	01	32.04
1. PDF card 28-1609 [Owen et al., 1972]	2.704	2	1	3	4	33.10
	2.681	3	0		5	33.40
References	2.662	3		2		33.64
Gabe, E. J. and Barnes, W. H. (1963). Acta	2.635	1	0		7	34.00
Crystallogr. <u>16</u> , 796.	2.5962	2	0	1	8	34.52
International Tables for X-ray Crystallography						
III (1962). (The Kynoch Press, Birmingham,	2.5532	7	0	4	1+	35.12
Eng.) p. 202.	2.5295	11	1	3	5+	35.46
Owen, J. T. R., Sithiraks, R., and Underwood,	2.4901	7		2	7+	36.04
F. A. (1972). J. Ass. Off. Anal. Chem. <u>55</u> ,	2.4768	6	0	3	6+	36.24
1171.	2.4558	2	1	1	8+	36.56

L-Cocaine Hydrochloride, $C_{17}H_{22}C1NO_4$ - (continued)

d(A)	I	ì	akl	λ -	2Θ(°) ο 1.540598A	
2.4238	1	1	4 1		37.06	
2.4063	2	3	1 2		37.34	
2.3553	1	1	3 6		38.18	
2.3283	9	2	1 7	+	38.64	
2.3088	6	1	4 3		38.98	
2.3053	6	2	3 4		39.04	
2.2707	3	1	2 8		39.66	
2.2436	2	3	1 4		40.16	
2.2224	2	1	1 9	+	40.56	
2.1904	9	2	0 8	+	41.18	
2.1732	6	3	2 3		41.52	
2.1682	6	2	2 7		41.62	
2.1407	1	3	1 5		42.18	
2.1349	1	2	4 0		42.30	
2.0999	2	0	1 10	+	43.04	
2.0733	1	3	0 6	+	43.62	
2.0661	2	1	0 10		43.78	
2.0439	3	3	3 0	+	44.28	
2.0326	5	3	1 6	+	44.54	
2.0188	4	2	2 8		44.86	
1.9804	4	1	5 1	+	45.78	
1.9618	7	2	3 7	+	46.24	
1.9233	3	3	2 6	+	47.22	
1.9172	4	0	1 11	+	47.38	
1.9111	4	2	4 5	+	47.54	
1.8968	2	1	3 9		47.92	
1.8575	2	0	5 5	+	49.00	
1.8455	4	3	3 5	+	49.34	
1.8413	3	2	1 10		49.46	
1.8330	2	2	4 6		49.70	
1.8145	1	4	1 3	+	50.24	
1.8045	3	1	4 8	+	50.54	
1.7847	2	0	5 6	+	51.14	
1.7750	2	3	3 6		51.44	
1.7705	2	4	1 4	+	51.58	
1.7572	2	2	5 3	+	52.00	
1.7540	2	3	4 3	+	52.10	
1.7379	1	2	0 11	+	52.62	
1.7132	3	2	1 11	+	53.44	
1.6973	1	4	2 4		53.98	

Cal	culated P	attern	(In	teg	rated)
d(Å)	Ι		hkl		2Θ(°) λ - 1.540598Å
10.73	100	0	0	2	8.23
9.29	54	0	1	1	9.52
7.43	20	0	1	2	11.90
7.19	31	1	0	1	12.30
6.220	2	1	0	2	14.23

I	hkl	2Θ(°) λ - 1.540598A
7	1 1 0	14.43
50	1 1 1	15.01
51	0 1 3	15.07
37	1 1 2	16.64
5	1 0 3	16.97
25	0 2 0	17.20
9	0 2 1	17.70
69	0 1 4	18.63
35	1 1 3	19.05
30	0 2 2	19.10
27	1 0 4	20.22
34	1 2 0	20.79
20	1 2 1	21.20
1	0 2 3	21.24
22	1 1 4	21.99
36	1 2 2	22.39
2	2 0 0	23.29
1	2 0 1	23.66
5	1 0 5	23.76
4	0 2 4	23.93
11	1 2 3	24.26
4	2 0 2	24.74
40	2 1 0	24.86
1	0 0 6	24.87
3	2 1 1	25.21
42	1 1 5	25.31
20	2 1 2	26.23
1	2 0 3	26.45
19	1 2 4	26.66
2	0 2 5	27.02
5	0 3 2	27.25
17	1 0 6	27.52
5	2 1 3	27.85
14	1 3 0	28.48
2	2 0 4	28.68
12	1 3 1	28.79
40	1 1 6	28.87
15	2 2 0	29.10
7	2 2 1	29.40
11	1 2 5	29.49
13	1 3 2	29.70
12	2 1 4	29.99
14	2 2 2	30.29
6	0 2 6	30.40
1	1 3 3	31.15
7 4 1 8 2	2 2 3 2 1 5 1 1 7 1 2 6 1 3 4	31.72 32.55 32.63 32.63
	7 50 51 37 5 25 9 69 35 30 27 34 20 1 22 36 2 1 5 4 11 4 40 1 3 42 20 1 19 2 5 17 5 14 2 12 40 15 7 11 13 12 14 6 1	7

L-Cocaine Hydrochloride, $C_{17}H_{22}ClNO_4$ - (continued)

d(A)	I		hkl		2θ(°) λ - 1.540598A
2.681 2.662	3	0 2	3 2	5 4	33.39 33.64
2.634	1	0	2	7	34.00
2.5959	2	0	1	8	34.52
2.5752	1	0	4	0	34.81
2.5569	6	0	4	1	35.07
2.5526	3	2	3	0	35.13
2.5347	1	2	3	1	35.38
2.5298 2.5297	6 7	2 1	1 3	6 5	35.45 35.46
2.4950 2.4902	3 5	2 1	2	5 7	35.97 36.04
2.4833	1	2	3	2	36.14
2.4770	3	0	3	6	36.24
2.4757	2	3	0	2	36.26
2.4701	1	3	1	0	36.34
2.4577	1	1	1	8	36.53
2.4539	1	3	1	1	36.59
2.4245	1	1	4	1	37.05
2.4071	2	3	1	2	37.33
2.3560	1	1	3	6	38.17
2.3348	2	3	1	3	38.53
2.3282	5	2	1	7	38.64
2.3280	5 1	2	2	6 4	38.65
2.3216	1	U	4	4	38.76
2.3094	5	1	4	3	38.97
2.3050	3	2	3	4	39.05
2.2989	2	3	0	4	39.15
2.2714	4	1	2	8	39.65
2.2437	2	3	1	4	40.16
2.2224	2	1	1	9	40.56
2.2212	1	1	4	4	40.58
2.1946	6	2	0	8	41.10
2.1939	1 5	2	3	5 7	41.11 41.17
2.1906	5	1			
2.1887	1	3	0	5	41.21
2.1733	6	3	2	3	41.52
2.1680	3	2	2	7	41.62
2.1409	1	3	1	5	42.18
2.1347	1	2	4	0	42.30
2.1009	2	0	1	10	43.02
2.0733	1	3	0	6	43.62
2.0659	2	1	0	10	43.78
2.0443 2.0372	2	3 1	3	0 8	44.27 44.43
			2		
2.0351	2	3	3 1	1	44.48 44.54
2.0325 2.0190	4	2	2	8	44.86
2.0190	1	3	3	2	45.11
1.9843	1	2	1	9	45.68
		_		Ū	

d(A)	I	hkl	2Θ(°) λ - 1.540598A
1.9809	1	0 2 10	45.77
1.9805	2	1 5 1	45.78
1.9797	2	0 5 3	45.80
1.9656	5	3 3 3	46.14
1.9616	6	2 3 7	46.24
1.9233	2	3 2 6	47.22
1.9174	1	1 2 10	47.37
1.9168	1	0 1 11	47.39
1.9163	1	1 5 3	47.40
1.9114	2	2 4 5	47.53
1.8971	2	1 3 9	47.91
1.8591	1	1 1 11	48.96
1.8573	1	0 5 5	49.01
1.8483	2	4 1 2	49.26
1.8456	3	3 3 5	49.34
1.8405	1	2 1 10	49.48
1.8331	2	2 4 6	49.70
1.8171	1	3 1 8	50.16
1.8149	1	4 1 3	50.23
1.8050	3	1 4 8	50.52
1.8035	2	3 4 1	50.57
1.7894	1	4 2 0	51.00
1.7852	1	0 5 6	51.12
1.7832	1	4 2 1	51.19
1.7748	1	3 3 6	51.45
1.7711	1	4 1 4	51.56
1.7574	1	2 5 3	51.99
1.7547	2	3 4 3	52.08
1.7519	1	2 4 7	52.17
1.7129	2	2 1 11	53.45
1.6975	1	4 2 4	53.97

Codeine Hydrobromide
Synonyms 1. 7,8-Didehydro-4,5-α-epoxy-3-methoxy-17- methyl-morphinan-6-α-ol hydrobromide hydrate 2. Methyl morphine hydrobromide hydrate
Structure Orthorhombic, P2 ₁ 2 ₁ 2 ₁ (19), Z = 4 [Lindsey and Barnes, 1955]. The structure was refined by Kartha et al. [1962]. The final R was 0.126. Intensities have been rounded to the nearer multiple of 10.
Atom positions C, O, and N atoms were all in general positions 4(a). The Br atom was represented by 2 isotropic half-atoms separated slightly along "x". The H atom positions were not determined [Kartha et al. 1962].
Lattice constants a = 13.090(10) Å b = 20.826(15) c = 6.808(5)
a/b = 0.6285 c/b = 0.3269
(published values: a = 13.089(10) Å, b = 20.825(15), c = 6.808(5) [Kartha et al.])
Volume 0 1856. Å ³
Density (calculated) 1.490 g/cm ³ (measured) 1.489 [Lindsey and Barnes, 1955]
Thermal parameters Isotropic [Kartha et al., 1962]
Scattering factors Zero ionization [International Tables, 1962]
Scale factor (integrated intensities) $\gamma = 0.4209 \times 10^{-3}$
Additional pattern 1. PDF card 10-801 [Barnes and Lindsey, 1955]
References Barnes, W. H. and Lindsey, J. M. (1955). Can. J. Chem. 33, 5674. International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 211. Kartha, G., Ahmed, F. R. and Barnes, W. H. (1962). Acta Crystallogr. 15, 326. Lindsey, J. M. and Barnes, W. H. (1955). Acta Crystallogr. 8, 227.

Calo	ulated	Pattern	(Pe	ak heig	ghts)
d(Å)	I		hkl	λ -	20(°) 。 - 1.540598A
10.39	20	0	2	0	8.50
8.14	20	1	2	0	10.86
6.47	10	0	1	1	13.68
6.24	20	2	1	0	14.18
6.13	20	1	3	0	14.44
6.04 5.79 5.70 5.22 4.83	50 40 50 90 30	1 1 0 1	0 1 2 2 4	1 1 1 1+ 0	14.66 15.28 15.54 16.98 18.34
4.72 4.60 4.55 4.27 4.13	60 10 10 1	2 2 1 3 0	0 1 3 1 4	1 1 1 0 1	18.80 19.28 19.48 20.78 21.48
4.02	10	3	2	0	22.08
3.942	100	1	4	1	22.54
3.904	20	2	3	1	22.76
3.616	20	3	1	1	24.60
3.551	1	0	5	1	25.06
3.496	30	2	4	1	25.46
3.466	10	3	2	1+	25.68
3.427	10	1	5	1	25.98
3.404	10	0	0	2	26.16
3.358	40	0	1	2+	26.52
3.271	10	4	0	0	27.24
3.234	10	0	2	2+	27.56
3.140	20	1	2	2	28.40
3.123	40	2	5	1+	28.56
3.056	1	0	3	2	29.20
3.002	20	3	4	1+	29.74
2.976	10	1	3	2	30.00
2.951	1	4	0	1	30.26
2.919	10	4	1	1	30.60
2.901	10	2	2	2	30.80
2.848	10	0	4	2	31.38
2.795	20	2	6	1	32.00
2.769	30	2	3	2+	32.30
2.714	20	4	3	1+	32.98
2.684	1	3	0	2	33.36
2.668	10	1	7	1	33.56
2.635	1	0	5	2	34.00
2.598	20	3	2	2+	34.50
2.566	1	4	4	1	34.94
2.553	1	1	8	0	35.12
2.517	1	2	7	1+	35.64
2.504	1	3	3	2	35.84
2.457	1	3	7	0	36.54
2.445	1	2	5	2	36.72
2.430	10	0	6	2+	36.96

Codeine Hydrobromide Hydrate, $C_{18}H_{22}BrNO_3 \cdot 2H_2O$ - (continued)

d(A)	I	hkl 2Θ(°) ° λ - 1.540598A
2.406	1	4 5 1 37.34
2.379	10	5 2 1+ 37.78
2.359	1	4 0 2 38.12
2.343	10	4 1 2 38.38
2.304	1	5 3 1 39.06
2.278	1	2 6 2+ 39.52
2.255	1	3 5 2 39.94
2.235	10	3 8 0 40.32
2.208	10	1 7 2+ 40.84
2.186	1	1 2 3+ 41.26
2.156	1	0 3 3 41.86
2.144	1	2 0 3+ 42.12
2.128	10	1 3 3+ 42.44
2.123	10	3 6 2+ 42.54
2.108	1	5 5 1 42.86
2.094	1	4 7 1 43.16
2.077	10	6 0 1+ 43.54
2.048	1	2 3 3+ 44.18
2.044	1	1 8 2+ 44.28
2.038	1	5 2 2+ 44.42
	_	
2.004	1	3 1 3 45.22
1.998	10	5 6 1 45.36
1.993	10	3 7 2+ 45.48
1.978	1	3 2 3 45.84
1.966	1	5 7 0 46.14
1.951	1	4 6 2 46.50
1.929	1	6 4 1+ 47.06
1.913	1	0 9 2 47.48
1.905	10	2 10 1+ 47.70
1.894	1	1 9 2 48.00
1.889	1	5 7 1 48.14
1.878	1	1 6 3+ 48.42
1.874	1	1 11 0 48.54
1.869	1	3 8 2 48.68
1.858	10	5 5 2 49.00
1.841	1	7 2 0 49.48
1.836	1	4 2 3+ 49.62
1.830	1	6 1 2 49.78
1.824	1	2 6 3 49.96
	-	

	Calculated	Pattern	(I	nte	grated)
d(A)	I		hkl	,	2Θ(°) ° λ - 1.540598A
10.41	20	0	2	0	8.48
8.15	20	1	2	0	10.85
6.55	1	2	0	0	13.52
6.47	10	0	1	1	13.67
6.24	20	2	1	0	14.17

d(Å)	Ι		hkl		2Θ(°) _o λ - 1.540598A
6.13 6.04	10 50	1 1	3	0	14.43 14.65
5.80	40	1	1	1 1	15.26
5.70	40	0	2	1	15.54
5.22	70	1	2	1	16.96
5.21	30	0	4	0	17.02
4.84	30	1	4	0	18.32
4.76	20	2	3	0	18.62
4.72 4.60	60 1	2 2	0	1	18.79 19.27
4.56	10	1	3	1	19.47
4.30	1	2	2	1	20.65
4.27	1	3	1	0	20.78
4.14	10	0	4	1	21.47
4.07	1	2	4	0	21.79
4.02	10	3	2	0	22.07
3.969 3.944	20 100	1 1	5 4	0	22.38 22.53
3.902	20	2	3	1	22.77
3.618	20	3	1	1	24.59
3.553	1	0	5	1	25.04
3.514	1	2	5	0	25.33
3.496	30	2	4	1	25.46
3.471 3.464	1 10	0 3	6 2	0	25.64 25.69
3.429	1	1	5	1	25.96
3.404	10	0	0	2	26.16
3.359	40	0	1	2	26.51
3.355	10	1	6	0	26.55
3.344	10	3	4	0	26.63
3.273	10	4	0	0	27.23
3.254	1	1	1	2	27.39
3.247 3.236	1 1	3 0	3	1 2	27.45 27.55
3.233	1	4	2 1	0	27.57
3.141	20	1	2	2	28.39
3.123	30	2	5	1	28.56
3.122	10	4	2	0	28.57
3.056 3.009	1 10	0 1	3 6	2	29.20 29.66
3.002	10	3	4	1	29.74
2.989	1	2	1	2	29.87
2.976	10	1	3	2	30.00
2.960	1	4	3	0	30.17
2.949	1	4	0	1	30.28
2.920	10	4	1	1	30.59
2.900	10	2	2	2	30.80
2.849	10	0	4	2	31.37
2.838 2.796	1 30	4 2	2 6	1 1	31.50 31.98

Codeine Hydrobromide Hydrate, $C_{18}H_{22}BrNO_3 \cdot 2H_2O$ - (continued)

d(Å)	I		hkl	λ - 1	2Θ(°) 。 .540598A
2.784 2.771 2.769 2.755 2.726	10 20 5 10	1 4 2 3 0	4 3 5	2 0 2 1	32.13 32.28 32.30 32.47 32.83
2.716 2.715 2.708 2.684 2.669	10 10 10	3 4 2 3 1	3 7 0	0 1 0 2 1	32.95 32.97 33.05 33.36 33.55
2.662 2.636 2.612 2.599 2.598	1 2 1 3	3 0 2 3 5	5 4 2	2 2 2 2 0	33.64 33.99 34.30 34.48 34.50
2.584 2.566 2.553 2.539 2.523	5 1 3 1 9 1	1 4 1 5 3	4 8 2	2 1 0 0 1	34.69 34.93 35.12 35.32 35.55
2.517 2.503 2.458 2.445 2.430	3 1 3 1 5 1	2 3 3 2 0	3 7 5	1 2 0 2 2	35.65 35.84 36.52 36.73 36.96
2.427 2.407 2.397 2.389 2.386	7 1 1 1 9 1	5 4 1 1 3	5 8 6	1 1 1 2 2	37.01 37.33 37.59 37.61 37.68
2.381 2.379 2.359 2.344 2.305	10 1 4 10	4 5 4 4 5	2 0	0 1 2 2 1	37.75 37.79 38.12 38.37 39.05
2.278 2.256 2.236 2.217 2.217	5 1 5 10 7 1	2 3 3 0 5	5 8 2	2 2 0 3 0	39.52 39.93 40.31 40.66 40.67
2.212 2.208 2.193 2.186 2.182	3 1 1 1 5 1	5 1 0 1 2	4 7 9 2 9	1 2 1 3 0	40.76 40.84 41.17 41.26 41.35
2.15 2.14 2.14 2.13 2.12	9 1 4 1 3 10	0 4 2 2 1	3 4 0 1 3	3 2 3 3 3	41.85 42.01 42.11 42.34 42.44

d(A)	Ι	hkl	2Θ(°) ° λ - 1.540598A
2.124 2.123 2.119	1 1 1	3 6	1 42.53 2 42.54 2 42.62
2.108 2.100	1 1	5 5	1 42.87 3 43.04
2.095 2.083 2.081 2.078	1 1 1 1	0 10	1 43.15 0 43.42 0 43.44 1 43.53
2.078	1	2 9	1 43.53
2.075 2.067 2.065 2.057 2.055	1 1 1 1	6 1 5 1 1 10	2 43.58 1 43.75 2 43.80 0 43.99 3 44.04
2.053 2.049 2.044 2.043 2.037	1 1 1 1	2 3 3 9 1 8	2 44.08 3 44.17 0 44.27 2 44.31 1 44.43
2.035 2.004 1.998 1.993 1.990	1 1 1 10 1	3 1 5 6	2 44.48 3 45.21 1 45.35 2 45.48 1 45.54
1.983 1.977 1.965 1.951	1 1 1 1	3 2 5 7 4 6	3 45.73 3 45.87 0 46.15 2 46.51 3 46.95
1.930 1.914 1.906 1.905 1.894	1 1 1 10 1	2 5	1 47.06 2 47.47 3 47.67 1 47.69 2 48.01
1.888 1.880 1.878 1.874 1.869	1 1 1 1	5 7 1 6 3 4 1 11 3 8	1 48.15 3 48.38 3 48.44 0 48.55 2 48.69
1.857 1.841 1.836 1.830 1.824	10 1 1 1 1	5 5 7 2 4 2 6 1 2 6	2 49.00 0 49.48 3 49.62 2 49.80 3 49.96

Structure Tetragonal, P4mbc (135), Z = 4. The structure was determined by Pertlik [1975].
Atom positions [Pertlik, 1975]
4(d) 4 copper 8(g) 8 oxygen(1) 8(h) 8 oxygen(2) 8(h) 8 arsenic
Lattice constants a = 8.592(4) Å c = 5.573(4) [ibid.]
a/c = 0.6486
Volume 6 411.4 Å ³
Density (calculated) 4.478 g/cm ³
Thermal parameters Isotropic, in table 3 [Pertlik, 1975]
Scattering factors Zero ionization [International Tables, 1962]
Scale factor (integrated intensities)
γ = 1.112 x 10 ⁻³ I/I corundum (calculated) = 4.16 for reflection with hk ℓ = 211.
References International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204, 211. Pertlik, F. (1975). Tschermak's Mineral. Petrogr. Mitt. 22, 211.

					
	lculated	Pattern	(Pea	k he	ights)
d(Å)	Ι		hkl	λ	2θ(°) 。 - 1.540598A
6.07 4.30 3.841 3.401 3.162	67 15 8 3 100	1 2 2 2 2	1 0 1 0 1	0 0 0 1	14.58 20.66 23.14 26.18 28.20
3.038	48	2	2	0	29.38
2.786	6	0	0	2	32.10
2.717	34	3	1	0	32.94
2.532	15	1	1	2	35.42
2.4416	1	3	1	1	36.78
2.3376	33	2	0	2	38.48
2.2554	14	2	1	2	39.94
2.1914	3	3	2	1	41.16
2.1475	1	4	0	0	42.04
2.0833	2	4	1	0	43.40
2.0536	2	2	2	2	44.06
2.0044	6	4	0	1	45.20
1.9514	30	4	1	1	46.50
1.9210	7	4	2	0	47.28
1.8159	3	4	2	1	50.20
1.8118	3	3	2	2	50.32
1.7185	1	4	3	0	53.26
1.7014	10	4	0	2	53.84
1.6721	11	2	1	3	54.86
1.6381	21	3	3	2	56.10
1.6128 1.5819 1.5336 1.5186 1.4734	1 1 1 1 8	5 4 5 4 5	1 2 2 4 3	1 2 1+ 0	57.06 58.28 60.30 60.96 63.04
1.4626	3	4	3	2	63.56
1.4420	12	5	1	2	64.58
1.4321	4	6	0	0	65.08
1.4247	3	5	3	1	65.46
1.4124	4	6	1	0	66.10
1.4053	2	4	0	3	66.48
1.3931	5	0	0	4	67.14
1.3869	9	4	1	3	67.48
1.3694	1	6	1	1	68.46
1.3579	1	1	1	4	69.12
1.3420	1	5	4	0	70.06
1.3337	2	4	4	2+	70.56
1.3197	1	6	2	1	71.42
1.3046	2	5	4	1	72.38
1.3027	2	5	3	2	72.50
1.2665	3	2	2	4	74.92
1.2599	2	6	1	2	75.38
1.2398	4	3	1	4	76.82
1.2211	5	6	2	2	78.22
1.2151	2	7	1	0+	78.68

d(Å)	I]	hkl		2Θ(°) 。 λ - 1.540598A
1.2090	2	5	4	2	79.16
1.1914	1	6	4	0	80.56
1.1546	2	7	2	1+	83.70
1.1280	2	4	2	4+	86.14
1.1137	2	5	5	2+	87.52
1.1057	2	7	3	1	88.32
1.0877	1	5	4	3	90.18
1.0792	1	6	5	1	91.08
1.0705	2	2	1	5	92.04
1.0656	1	8	1	0	92.58
1.0466	2	7	4	1+	94.78
1.0458	2	7	3	2	94.88
1.0420	2	8	2	0	95.34
1.0233	1	6	5	2	97.66

	Calculated	Patte	rn	(In	tegrated)
d(Å)	I		hkl		2Θ(°) ο λ - 1.540598A
6.08	58	1	1	0	14.57
4.30	14	2	0	0	20.66
3.842	8	2	1	0	23.13
3.402	3	2	0	1	26.17
3.163	100	2	1	1	28.19
3.038	48	2	2	0	29.38
2.787	6	0	0	2	32.10
2.717	35	3	1	0	32.94
2.533	15	1	1	2	35.41
2.4422	1	3	1	1	36.77
2.3378	35	2	0	2	38.48
2.2558	15	2	1	2	39.93
2.1911	3	3	2	1	41.17
2.1480	1	4	0	0	42.03
2.0839	2	4	1	0	43.39
2.0534	2	2	2	2	44.06
2.0043	7	4	0	1	45.20
1.9519	34	4	1	1	46.49
1.9453	1	3	1	2	46.65
1.9212	7	4	2	0	47.27
1.8163	3	4	2	1	50.19
1.8110	2	3	2	2	50.34
1.7184	1	4	3	0	53.26
1.7012	11	4	0	2	53.85
1.6725	13	2	1	3	54.85
1.6382	24	3	3	2	56.10
1.6129	1	5	1	1	57.06
1.5817	2	4	2	2	58.29
1.5339	1	5	2	1	60.29
1.5189	1	4	4	0	60.95

0					
d(A)	I		hkl		2Θ(°)
					λ - 1.540598Α
1.4735	10	5	3	0	63.04
1.4651	1	3	2	3	63.44
1.4626	3	4	3	2	63.56
1.4419	14	5	1	2	64.58
1.4320	4	6	0	0	65.08
1.4246	3	5	3	1	65.47
1.4125	4	6	1	0	66.10
1.4051	2	4	0	3	66.49
1.3933	6	0	0	4	67.13
1.3869	1	6	0	1	67.48
1.3867	9	4	1	3	67.49
1.3846	1	5	2	2	67.61
1.3692	1	6	1	1	68.47
1.3580	1	1	1	4	69.11
1.3418	1	5	4	0	70.07
1.3355	1	4	2	3	70.45
1.3336	2	4	4	2	70.56
1.3199	1	6	2	1	71.41
1.3046	2	5	4	1	72.38
1.3026	2	5	3	2	72.51
1.2664	4	2	2	4	74.93
1.2599	2	6	1	2	75.38
1.2398	5	3	1	4	76.83
1.2211	7	6	2	2	78.22
1.2151	1	7	1	0	78.68
1.2090	2	5	4	2	79.16
1.1915	1	6	4	0	80.56
1.1546	ī	7	2	1	83.70
1.1544	1	5	3	3	83.71
1.1279	2	4	2	4	86.15
1.1138	2	5	5	2	87.51
1.1058	3	7	3	1	88.31
1.0878	1	5	4	3	90.17
1.0793	1	6	5	1	91.08
1.0705	2	2	1	5	92.04
1.0657	2	8	1	0	92.57
1.0467	1	7	4	1	94.77
1.0457	2	7	3	2	94.89
1.0419	2	8	2	0	95.34
1.0232	1	6	5	2	97.67

Synonyms	Ca
The name hartite was designated in 1841 and material called bombiccite was described later. Because of uncertainty in the chemistry, the two were not identified	d(A)
as the same phase until 1955 [Pellizer, 1955].	21.02 10.52 8.19
Structure Triclinic, P1 (1), Z = 4. The structure was determined by Serantoni et al. [1978]. The	7.14 6.99
natural mineral used for the determination was repeatedly dissolved and recrystallized from benzene.	6.64 6.16 6.02 5.84
Atom positions 1(a) 80 carbon Hydrogen positions were not specified.	5.52 5.45
Lattice constants $a = 11.39(7) \stackrel{\circ}{A}$ $b = 21.29(5)$	5.37 5.25 5.18 5.01
c = 7.45(1) $\alpha = 94.6(1)^{\circ}$ $\beta = 101.8(2)$ $\gamma = 81.5(1)$	4.92 4.89 4.64 4.56
a/b = 0.5350 c/b = 0.3499	4.52
Volume 1747. A ³	4.33 4.16 4.09 4.04
Density (calculated) 1.044 g/cm ³ (measured) 1.08 [Serantoni et al., 1978]	3.91
Thermal parameters Isotropic B _i calculated from U _i given in Serantoni et al. [1978]	3.78 3.75 3.68
Scattering factors	3.61 3.58 3.55
C ⁰ [Cromer and Mann, 1968] Scale factor (integrated intensities)	3.48 3.39
$\gamma = 3.162 \times 10^{-3}$ References Cromer, D. T. and Mann, J. B. (1968). Acta	3.37 3.36 3.33 3.22
Crystallogr. A24, 321. Pellizer, R. (1955). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 19, 150.	3.16
Serantoni, E. F., Krajewski, A., Mongiorgi, R., Riva di Sanseverino, L. and Sheldrick, G. M. (1978). Acta Crystallogr. <u>B34</u> , 1311.	3.06 3.01 2.98 2.92

	Calculated	Pattern	(Pea	k heig	hts)
d(A)	I		hkl	λ -	2Θ(°) ° 1.540598A
21.0 10.5 8.1 7.1 6.9	2 35 9 3 4 7	0 0 1 -1 0	1 2 2 2 -1	0 0 0 0 1	4.20 8.40 10.80 12.38 12.66
6.6 6.1 6.0 5.8 5.5	6 40 2 4 4 3	-1 -1 -1 0 2	-1 1 -2 2 0	1 1 1 1 0	13.32 14.36 14.70 15.16 16.04
5.4 5.3 5.2 5.1 5.0	7 45 5 9 8 13	1 1 0 2 1	1 -1 4 2 4	1 1 0 0+ 0+	16.26 16.50 16.86 17.10 17.70
4.9 4.8 4.6 4.5	9 3 4 5 6 6	-2 1 -2 -1	-1 -2 2 3 4	1 1+ 0 1	18.00 18.14 19.12 19.46 19.64
4.4 4.3 4.1 4.0 4.0	3 1 6 3 9 3	1 -2 0 2 2	3 -3 4 4 0	1+ 1 1 0 1+	20.04 20.50 21.34 21.72 22.00
3.9 3.8 3.7 3.7	9 2 8 1 5 1	2 -2 1 -2 2	-1 -4 -4 3 -2	1 1+ 1+ 1 1+	22.72 22.84 23.54 23.72 24.16
3.6 3.5 3.5 3.4 3.3	8 2 5 1 8 2	2 -2 -3 1 0	3 4 1 6 2	1+ 0+ 0 0 2+	24.64 24.88 25.08 25.60 26.30
3.3 3.3 3.2 3.1	6 1 3 2 2 1	-1 -2 -3 3 -1	5 0 2 4 -4	1+ 2 0+ 0+ 2+	26.40 26.54 26.78 27.68 28.22
3.1 3.0 3.0 2.9 2.9	6 4 1 2 8 1	-1 3 -2 3 0	3 1 -4 -1 4	2+ 1 2+ 1 2+	28.48 29.14 29.68 29.92 30.56
2.8 2.7 2.7 2.6 2.6	6 2 2 1 4 1	-1 4 -4 1 -2	4 0 -3 8 -6	2+ 0+ 1+ 0 2	30.98 32.38 32.88 33.96 34.50

d(Å)	Ι	hkl	2Θ(°) λ - 1.540598A
2.54 2.426 2.387 2.353 2.301	1 1 2 1	3 -4 1 4 0 1+ 4 -1 1+ -4 -4 2+ -1 -9 1+	35.26 37.02 37.66 38.22 39.12
2.281 2.259 2.214 2.200 2.162 2.119 2.091	1 1 1 1 1 2	-2 6 2+ 0 -9 1+ -1 -5 3+ -2 3 3+ -4 -6 2+ 1 10 0+ -3 -5 3+	39.48 39.88 40.72 41.00 41.74 42.64 43.24

	Calculated	Pattern	(In	tegrated)
d(A)	I	hks)	2Θ(°) 。
				λ - 1.540598A
21.03	5	0 1	0	4.20
10.51	35	0 2	0	8.40
8.19	3	1 2	0	10.80
7.15	6	-1 2	0	12.37
6.99	14	0 -1	1	12.65
6.77	1	0 1	1	13.06
6.65	45	-1 -1	1	13.30
6.17	45	-1 1	1	14.35
6.14	2	0 -2	1	14.42
6.02	3	-1 -2	1	14.70
5.85	2	0 2	1	15.14
5.60	5	1 0	1	15.82
5.53	5	2 1	0	16.02
5.52	100	2 0	0	16.03
5.45	45	1 1	1	16.25
5.37	45	1 -1	1	16.49
5.35	1	- 1 2	1	16.55
5.26	6	0 4	0	16.85
5.20	2	- 1 - 3	1	17.05
5.19	6	2 2	0	17.08
5.19	2	0 -3	1	17.08
5.17	3	- 2 1	0	17.12
5.02	3 5	1 4	0	17.67
5.00	5	1 2	1	17.72
4.93	4	-2 -1	1	17.99
4.88	1	- 2 0	1	18.15
4.88	2	1 -2	1	18.15
4.65	1	2 3	0	19.05
4.64	5	-2 2	0	19.11
4.60	1	- 2 1	1	19.26

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
4.56 4.52 4.44 4.43 4.33	6 6 2 1 1	-1 3 1 -1 4 0 1 3 1 -1 -4 1 -2 -3 1	19.44 19.64 20.00 20.04 20.48
4.16 4.09 4.08 4.04 3.91	3 3 1 1 3	0 4 1 2 4 0 -2 3 0 2 0 1 2 -1 1	21.33 21.69 21.77 22.00 22.70
3.89 3.78 3.75 3.68 3.64	1 1 1 1	-2 -4 1 1 -4 1 -2 3 1 2 -2 1 0 0 2	22.85 23.52 23.73 24.14 24.43
3.61 3.58 3.55 3.48 3.36	1 2 1 3 1	2 3 1 -2 4 0 -3 1 0 1 6 0 -2 0 2	24.65 24.88 25.08 25.59 26.53
3.34 3.32 3.16 3.13 3.08	1 1 1 1	-3 2 0 -2 -2 2 -1 -4 2 -1 3 2 -2 2 2	26.68 26.79 28.20 28.45 28.93
3.06 3.05 3.01 2.98 2.92	5 1 1 1	3 1 1 3 0 1 -2 -4 2 3 -1 1 0 4 2	29.14 29.21 29.64 29.91 30.55
2.90 2.89 2.76 2.76 2.64	1 3 1 1	3 3 1 -1 4 2 -3 4 1 4 0 0 1 8 0	30.83 30.97 32.35 32.39 33.95
2.60 2.54 2.387 2.386 2.317	1 1 1 1	-2 -6 2 3 -4 1 -3 4 2 4 -1 1 4 -2 1	34.50 35.26 37.65 37.66 38.84
2.281 2.214 2.200 2.091	1 1 1 1	-2 6 2 -1 -5 3 -2 3 3 -3 -5 3	39.47 40.71 41.00 43.24

(-)-Ephedrine Hydrochloride, $C_{10}H_{16}ClNO$

Synonyms 1. Biophedrin 2. Ephedral 3. Sanedrine	
CAS registry no. 877-36-1	
Structure Monoclinic, P2 ₁ (4), Z = 2. The structure was determined by Phillips [1954]. Bergin [1971] refined the structure using 3-dimensional data.	!
Atom positions All atoms were in general positions 2(a) [Bergin, 1971].	
Lattice constants Bergin [1971] a = 12.671(3) Å b = 6.090(4) c = 7.301(2) β = 102.11(8)°	
a/b = 2.0806 c/b = 1.1989	
Volume o 550.9 A ³	
Density (calculated) 1.216 g/cm ³	
Thermal parameters Anisotropic [Bergin, 1971]	
Scattering factors Zero ionization [International Tables, 1962]	
Scale factors (integrated intensities) $\gamma = 0.6728 \times 10^{-3}$ I/I corundum (calculated) = 0.962 for reflection with hk ℓ = 011.	
Additional patterns 1. PDF card 5-0263 [E. Lilly and Co., Indianapolis, IN] 2. PDF card 24-1735 [Institute of Physics, University College, Cardiff, Wales]	
References Bergin, R. (1971). Acta Crystallogr. <u>B27</u> , 381. International <u>Tables for X-ray Crystallography</u> III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Phillips, D. C. (1954). Acta Crystallogr. <u>7</u> , 159.	

	Calculated	Pattern	(Pea	ak heights)
d(Å)	I	ŀ	ıkl	2Θ(°) ° λ - 1.540598A
12.37 7.13 6.84 6.19 5.68	9 17 45 4 9	1 0 -1 2 1	0 0 0 1 0 1 0 0 0 1	1 12.40 1 12.94 0 14.30
5.46 4.629 4.544 4.341 4.130	15 100 21 18 25	1 0 -1 2 3	1 1	1 19.16 1 19.52 0 20.44
3.976 3.952 3.636 3.567 3.488	4 4 2 27 10	-2 -3 -1 0 2	0 1 0 2 0 2	1 · 22.34 1 22.48 2 24.46 2 24.94 1 25.52
3.417 3.314 3.123 3.079 3.046	35 9 5 20 3	3 -3 -1 0	1 1 1 2 1 2	0+ 26.06 1 26.88 2 28.56 2 28.98 0 29.30
2.980 2.957 2.893 2.868 2.781	18 6 9 13 5	-2 1 3 1 -1	2 (1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2	2 29.96 0 30.20 1 30.88 2 31.16 1 32.16
2.754 2.733 2.715 2.684 2.635	9 3 6 4 5	-4 2 -3 1 -2	2 (1 2 2 1	1+ 32.48 0 32.74 2 32.96 1 33.36 1 34.00
2.577 2.477 2.426 2.413 2.396		2 2 4 -3 -2	2 1 1 2	2 34.78 1 36.24 1 37.02 1+ 37.24 3 37.50
2.379 2.335 2.317 2.295 2.273	1 1 1	0 -1 -5 5 -2	2 2 1 1 1 1 1	3 37.78 2 38.52 1+ 38.84 0 39.22 2 39.62
2.260 2.252 2.230 2.171 2.148	. 2 5 2	-1 1 -2 4 -3	0 : 1 : 2 :	3 39.86 3 40.00 3+ 40.42 0 41.56 2 42.02
2.134 2.129 2.105 2.079 2.009	3 3 2	-3 4 -6 2 4	0 2 2 2	3 42.32 2+ 42.42 1 42.94 2 43.50 2 45.10

(-)-Ephedrine Hydrochloride, $C_{10}H_{16}C1N0$ - (continued)

2.004 2 1 3 0 45.22 1.998 2 4 2 1+ 45.36 1.990 1 -6 1 1+ 45.54 1.975 1 -6 0 2 45.90 1.955 2 6 1 0 46.40 1.947 1 -1 3 1 46.62	
1.990 1 -6 1 1+ 45.54 1.975 1 -6 0 2 45.90 1.955 2 6 1 0 46.40	
1.975 1 -6 0 2 45.90 1.955 2 6 1 0 46.40	
1.955 2 6 1 0 46.40	
1.947 1 -1 3 1 46.62	
1.929 1 2 3 0 47.08	
1.912 1 3 2 2+ 47.52	
1.901 1 -1 2 3 47.82	
1.881 4 6 0 1+ 48.36	
1.876 3 0 2 3 48.48	
1.840 1 -5 1 3 49.50	
1.832 1 2 3 1 49.72	
1.821 2 3 3 0+ 50.06	
1.810 1 1 2 3+ 50.38	
1.744 2 -2 1 4+ 52.42	
1.731 1 -6 2 1 52.84	
1.721 2 4 0 3+ 53.18	
1.713 2 0 1 4 53.46	
1.696 1 -4 3 1+ 54.02	
1.683 1 -6 1 3 54.46	
1.652 1 1 1 4+ 55.58	
1.578 1 -5 3 1 58.42	
1.562 2 -2 2 4+ 59.10	

		Calculated	Patte	rn	(In	tegrated)
	d(A)	I		hks	2	2Θ(°) λ - 1.540598A
	12.39	8	1	0	0	7.13
	7.14	15	0	0	1	12.39
	6.84	43	-1	0	1	12.94
	6.19	3	2	0	0	14.29
	5.69	8	1	0	1	15.56
	5.47	14	1	1	0	16.20
	4.633	100	0	1	1	19.14
	4.547	18	-1	1	1	19.50
	4.343	18	2	1	0	20.43
	4.158	8	1	1	1	21.35
	4.130	24	3	0	0	21.50
1	3.979	3	-2	1	1	22.32
	3.952	3	-3	0	1	22.48
	3.639	1	-1	0	2	24.44
	3.569	28	0	0	2	24.93
	3.489	10	2	1	1	25.51
	3.418	14	-2	0	2	26.05
	3.418	23	3	1	0	26.05
	3.315	9	-3	1	1	26.87
	3.124	4	-1	1	2	28.55

d(A)	I		hkl		2Θ(°) 。
					λ - 1.540598Å
3.097	4	4	0	0	28.80
3.088 3.079	1 20	-4 0	0 1	1 2	28.89 28.97
3.045	20	0	2	0	29.31
2.981	20	-2	1	2	29.95
2.957	5	1	2	0	30.20
2.893	9	3	1	1	30.88
2.869	14	1	1	2	31.15
2.782 2.761	5 3	-1 4	2	1 0	32.15 32.40
2.754	7	-4	1	1	32.49
2.733	2	2	2	0	32.75
2.715	6	- 3	1	2	32.96
2.685	4	1	2	1	33.35
2.646	2	4	0	1	33.85
2.635 2.578	5 2	-2 2	2	1 2	34.00 34.77
2.477	4	2	2	1	36,24
2.433	1	-1	0	3	36.91
2.427	4	4	1	1	37.01
2.413	1	-4	1	2	37.23
2.412	5	-3	2	1	37.25
2.396 2.380	1 4	-2 0	0	3	37.51 37.78
2.335	1	-1	2	2	38.52
2.295	1	5	1	0	39.22
2.279	1	- 3	0	3	39.51
2.274	6	-2	2	2	39.61
2.260 2.251	2 1	-1 1	1 0	3 3	39.86 40.02
2.234	3	3	2	1	40.34
2.230	3	-2	1	3	40.42
2.171	2	4	2	0	41.56
2.149	3	-3	2	2	42.01
2.134	2	-3	1	3	42.31
2.129	1	4	0	2	42.43
2.105	3	-6	0	1	42.93
2.079 2.009	3 1	2 4	2 1	2 2	43.50 45.08
2.003	1	1	3	0	45.23
1.997	1	4	2	1	45.37
1.989	1	-6	1	1	45.56
1.976	1	-6	0	2	45.89
1.955 1.946	3 1	6 -1	1 3	0 1	46.40 46.64
1.929 1.901	1 1	2 -1	3 2	0 3	47.07 47.81
1.883	2	-2	2	·3	48.30
1.881	2	6	0	1	48.35
1.880	1	-6	1	2	48.39

(-)-Ephedrine Hydrochloride, $C_{10}H_{16}ClNO$ - (continued)

d(Å)	I	hkl 2θ(°) ° λ - 1.540598A
1.875 1.840 1.832 1.825 1.822	2 1 1 1	0 2 3 48.52 -5 1 3 49.49 2 3 1 49.72 -3 2 3 49.95 3 3 0 50.03
1.820 1.810 1.745 1.743 1.731	1 1 1 1	-5 2 2 50.07 1 2 3 50.37 -2 3 2 52.38 -2 1 4 52.45 -6 2 1 52.83
1.722 1.721 1.713 1.696 1.684	1 1 2 1 2	1 3 2 53.14 4 0 3 53.19 0 1 4 53.46 -4 3 1 54.02 -6 1 3 54.45
1.578 1.564 1.562	1 1 2	-5 3 1 58.43 -5 1 4 59.02 -2 2 4 59.10

Synonyms 1. Haldol 2. Serenase 3. 4-(4-hydroxy-4-p-chlorphenylpiperidino)4'- fluorobutyrophenone
CAS registry no. 52-86-8
Structure Monoclinic, $P2_1/c$ (14), $Z = 4$. The structure was refined by Reed and Schaefer [1973].
Atom positions All atoms were in general positions 4(e). The "x" parameter for carbon(7) was used as 0.0838. No hydrogen positions were listed in the ref- erence.
Lattice constants a = 7.816(5) Å b = 8.996(6) c = 28.346(20) β = 106.34°
(published values: a = 7.816(5)Å, b = 8.995(6), c = 28.344(20), β = 106.34(4)° [Reed and Schaefer, 1973])
CD cell: $a = 27.202$, $b = 8.996$, $c = 7.816$, $\beta = 90.33^{\circ}$, space group $P2_1/n$; $a/b = 3.0237$, $c/b = 0.8688$
Volume o 1912.6 A ³
Density (calculated) 1.305 g/cm ³ (measured) 1.23 g/cm ³ [Reed and Schaefer, 1973]
Thermal parameters Anisotropic [Reed and Schaefer, 1973]
Scattering factors Zero ionization [International Tables, 1962]
Scale factor (integrated intensities) $\gamma = 1.271 \times 10^{-3}$ I/I corundum (calculated) = 1.29 for reflection
with $hk\ell = \overline{1}15$.
References International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Reed, L. L. and Schaefer, J. P. (1973). Acta Crystallogr. <u>B29</u> , 1886.

	ulated	Pattern	(Pea	k l	heights)	
d(A)	I		hkl		2Θ(°) λ - 1.54059	o 8Å
8.53 7.49 6.79 6.38 5.93	2 10 1 3 19	0 1 0 0 -1		1 0+ 4 3 4+	10.36 11.80 13.02 13.86 14.94	
5.76 5.41 4.946 4.653 4.467	5 6 2 3 100	-1 1 -1 0 -1	1 1 1	2+ 1+ 4+ 5	15.36 16.36 17.92 19.06 19.86	
4.044 3.897 3.751 3.584 3.464	1 13 3 11 1	0 -1 0 -1 2	2	6 1 4+ 4+ 0+		
3.396 3.339 3.177 3.000 2.986	7 2 6 6 5	-2 -2 -2 -2 2	0 1 1 1 1	6+ 5 6 7 3+	26.68 28.06 29.76	
2.951 2.934 2.881 2.808 2.784	2 3 3 4 3	-1 -2 2 -2	1 2 2 2 3	9+ 3+ 0+ 5+	30.44 31.02 31.84	
2.745 2.711 2.641 2.592 2.508	2 2 1 1	1 -2 -2 -2 0	2 2 1 2 2	6+ 6 9 7+ 9	33.02 33.92	
2.491 2.474 2.464 2.370 2.354	1 2 3 1 1	-1 -1 -3 -2 -2	3 1 1 1 3 2	6+ 1+ 5+ 1+ 9+	36.28 36.44 37.94	
2.345 2.248 2.226 2.129 2.119	2 1 1 1 1	-2 -2 2 0 -1	3 0 3 1 1	4+ 6+ 8+ 9	40.08	
2.113 2.103 2.010 1.955 1.947	1 1 3 1 2	1 -1 3 2 -3	4 1	1+ 4+ 5+ 10+ 5+	42.98 45.08 46.40	
1.907 1.873	1 1	-2 -2	4 3 1	5 l 1+	47.66 48.58	

${\it Haloperidol}, \; {\it C_{2\,1}H_{2\,3}ClFNO_2} \; \hbox{- (continued)}$

	Calculated	Pattern	(Inte	grated)
d(Å)	I	hk		20(°) 1.540598A
8.54	2	0 1	1	10.35
7.52	1	-1 0	2	11.75
7.50	3	0 1	2	11.79
7.50	6	1 0	0	11.79
6.80	1	0 0	4	13.01
6.39	3	0 1	3	13.86
5.94	15	-1 0	4	14.91
5.90	5	1 0	2	15.00
5.90	9	-1 1	1	15.00
5.77	3	-1 1	2	15.34
5.76 5.42 5.42 5.40 4.955	2 3 2 3 1	1 1 0 1 -1 1 1 -1 1	0 4 3 1 4	15.37 16.33 16.34 16.39 17.89
4.935	1	1 1	2	17.96
4.655	2	0 1	5	19.05
4.534	2	0 0	6	19.57
4.498	55	0 2	0	19.72
4.477	2	-1 0	6	19.81
4.466 4.048 3.908 3.899 3.762	100 1 1 13 1	-1 1 0 1 -2 0 -1 2 -2 0	5 6 2 1 4	19.86 21.94 22.74 22.79 23.63
3.752	2	0 2	4	23.70
3.603	4	-1 1	7	24.69
3.585	9	-1 2	4	24.81
3.578	3	1 2	2	24.87
3.400	1	0 0	8	26.19
3.397	6	-2 0	6	26.21
3.386	2	-1 2	5	26.30
3.378	1	1 2	3	26.36
3.339	2	-2 1	5	26.67
3.178	6	-2 1	6	28.06
3.165	2	1 2	4	28.18
3.000	7	-2 1	7	29.75
2.986	3	2 1	3	29.90
2.981	2	0 3	1	29.95
2.969	2	-2 0	8	30.08
2.941	1	0 2	7	30.37
2.934	2	-2 2	3	30.44
2.886	1	-2 2	4	30.96
2.880	2	2 2	0	31.02
2.813	2	1 0	8	31.78
2.809 2.786 2.784 2.756 2.748	2 1 3 1	-2 2 -1 3 1 3 -1 2 1 2	5 2 0 8 6	

d(A)	I	hkl	2Θ(°) 。
			λ - 1.540598A
	····		· · · · · · · · · · · · · · · · · · ·
2.711	2	- 2 2 6	33.02
2.642	1	-2 1 9	33.91
2.598	1	-2 2 7	34.49
2.509	1	0 2 9	35.76
2.474	2	-1 1 11	36.28
2.464	2	- 3 1 5	36.44
2.369	1	-2 3 1	37.95
2.345	2	-2 3 4	38.36
2.248	1	-2 3 6	40.08
2.226	1	2 0 8	40.48
2.129	1	0 3 9	42.43
2.119	1	-1 1 13	42.63
2.103	1	-1 4 4	42.97
2.010	2	3 1 5	45.07
2.007	1	1 4 4	45.13
	_		
1.956	1	2 0 10	46.39
1.948	1	-3 3 5	46.59
1.945	î	-2 4 3	46.67
1.907	1	-2 4 5	47.65
1.507	1	2 4 3	47.03
l			

	lculated	Pattern	(Pe	ak he	ights)
d(A)	I		hkl	λ	2Θ(°) - 1.540598 <i>E</i>
14.62	8	0	2	0	6.04
10.11	78	0	1	1	8.74
8.53	86	1	0	0	10.36
8.20 7.36	14 30	1 1	1 2	0 0+	10.78 12.02
7.23	77	0	3	1	12.24
7.13	46	-1	0	2	12.40
6.932	13	-1	1	2	12.76
6.104 5.757	2 8	-1 -1	4 3	1 2	14.50 15.38
5.549	47	1	4	0	15.96
5.460	97	-2	1	2	16.22
5.304	6	0	1	2	16.70
5.187 5.018	21 71	-2 -2	2	2+ 1	17.08 17.66
4.870	100	0	6	0	18.20
4.721	7	0	3	2	18.78
4.609	10	1	3	1	19.24
4.562	11	-2	1	3	19.44
4.432	40	- 2	4	2+	20.02
4.267	56	2	0	0+	20.80
4.172	35	-2	3	3	21.28
4.100	56	2	2	0+	21.66
4.030 3.942	7 10	-2 -2	5 5	2 1	22.04 22.54
3.907	17	2	3	0+	22.74
3.751	50	1	7	0	23.70
3.714	36	-3		2	23.94
3.684	39 39	2 -2	4 6	0+ 2	24.14 24.26
3.613 3.567	24 53	0 -2	6 0	2+ 4	24.62 24.94
3.545	24	-2	1	4	25.10
3.466	54	-2		4+	25.68
3.388	5	1	3	2	26.28
3.324	30	-1	6	3+	26.80
3.290 3.250	10 30	-2 -1	7 8	1+ 2+	27.08 27.42
3.207	27	-2		4	27.42
3.164	10	-3	3	1	28.18
3.129	10	- 3	5	3+	28.50
3.089	5	-1	3	4	28.88
3.074	6	1	5	2+	29.02
3.054 3.028	9 5	-2 0	8	2	29.22 29.48
2.974	5	-1	4	4	30.02
2.955	8	-1	9	2+	30.22
2.923	4	0	10	0	30.56
2.904	3	-3 -3	5 5	1+ 4+	30.76
2.093	3	-3	5	4 1	30.86

d(A)	I	hkl	2Θ(°) λ - 1.540598Å
2.866	5	-2 8 3	31.18
2.847	7	3 0 0+	31.40
2.826	4	-1 10 1	31.64
2.819	5	-3 1 5	31.72
2.776	7	2 8 0+	32.22
2.731	12	-4 2 4+	32.76
2.727	12	0 7 3+	32.82
2.704	11	-4 3 3+	33.10
2.699	11	0 0 4	33.16
2.673	3	-4 3 4	33.50
2.653	12	0 2 4+ -4 2 2 2 0 2+ -3 7 4+ 0 11 1+	33.76
2.630	5		34.06
2.617	5		34.24
2.602	8		34.44
2.579	4		34.76
2.552	3	1 10 1+ -3 5 5 0 4 4+ -4 5 4 -4 3 5	35.14
2.548	3		35.20
2.531	5		35.44
2.512	2		35.72
2.498	2		35.92
2.491	2	-1 11 2	36.02
2.478	1	1 5 3	36.22
2.458	2	3 6 0	36.52
2.431	3	-4 5 2+	36.94
2.411	2	1 9 2+	37.26
2.379	8	-2 11 1+	37.78
2.360	6	0 6 4	38.10
2.354	6	3 7 0	38.20
2.345	4	-4 6 2	38.36
2.325	4	3 3 1+	38.70
2.300	4	-1 9 4+	39.14
2.296	4	-4 4 1	39.20
2.283	2	-4 6 5+	39.44
2.274	2	1 10 2+	39.60
2.261	3	-5 0 4+	39.84
2.247	3	3 8 0+	40.10
2.233	3	-5 2 4+	40.36
2.215	4	3 5 1+	40.70
2.203	6	-1 13 1+	40.94
2.175	4	-5 2 3+	41.48
2.170	4	1 2 4+ -4 8 2+ 4 0 0+ -2 9 5+ -5 0 6+	41.58
2.158	2		41.82
2.135	6		42.30
2.121	6		42.60
2.107	3		42.88
2.084	7	-2 13 2+	43.38
2.079	6	-3 11 4+	43.50
2.072	5	-2 13 1	43.64
2.059	3	-5 1 2	43.94
2.050	4	-5 6 4+	44.14

d(Å)	I	hkl 20(°) ° λ - 1.540598A
2.044	4	- 5 2 2 44.28
2.039	3	2 9 2+ 44.40
2.021	4	- 4 9 5+ 44.80
2.013	4	- 4 2 7 + 45.00
1.999	2	1 6 4+ 45.32
1.987	2	3 3 2+ 45.62
1.955	3	4 6 0+ 46.40
1.945	3	-5 7 3+ 46.66
1.938	3	- 3 11 5+ 46.84
1.922	3	-3 13 2+ 47.26
1.918	4	0 15 1+ 47.36
1.907	3	0 13 3+ 47.64
1.902	2	-2 14 3+ 47.78
1.898	2	-1 14 3 47.88

	Calculated	Pattern	(In	tegrated)
d(Å)	I	hk	L	2Θ(°) ° λ ~ 1.540598A
14.61 10.40 10.13 8.54 8.20 7.38 7.33 7.23	7 3 73 81 12 19 10 66	0 2 -1 1 0 1 1 0 1 1 1 2 -1 3 0 3	1 1 0 0 0	6.04 8.50 8.73 10.35 10.78 11.99 12.07 12.23
7.14 6.934 6.107 5.758 5.553 5.464	34 10 1 7 40 93	-1 0 -1 1 -1 4 -1 3 1 4 -2 1	2 1 2 0	12.39 12.76 14.49 15.38 15.95 16.21
5.397 5.397 5.198 5.175 5.140 5.106	6 2 15 8 2 4	0 0 0 1 -2 2 -1 5 0 5 -1 4	2 2 2 1 1	16.41 16.69 17.04 17.12 17.24 17.35
5.063 5.021 4.872 4.824 4.721	13 67 100 5 5	0 2 -2 2 0 6 1 5 0 3	1 0 0	17.50 17.65 18.20 18.38 18.78
4.612 4.564 4.523 4.494 4.462	8 9 1 5 25	1 3 -2 1 -1 5 -1 1 -1 6	3 2	19.23 19.43 19.61 19.74 19.88

Imipramine Hydrochloride, $C_{19}H_{25}ClN_2$ - (continued)

d(A)	I	hkl λ -	2Θ(°) - 1.540598Å	d(Å)	I	hkl	2Θ(°) λ - 1.540598
4.440 4.426 4.406 4.315 4.271	20 21 2 9 44	0 6 1 -2 4 2 -2 2 3 -2 4 1 2 0 0	19.98 20.05 20.14 20.57 20.78	3.252 3.246 3.212 3.207 3.180	14 12 3 24	-1 8 2 -3 2 4 2 6 0 -2 4 4 -1 2 4	27.40 27.45 27.75 27.80 28.04
. 256 . 232 . 227 . 175 . 121	20 15 6 32 23	1 4 1 1 6 0 2 1 0 -2 3 3 -1 3 3	20.86 20.98 21.00 21.26 21.54	3.165 3.136 3.131 3.126 3.118	9 3 6 1 3	-3 3 1 -3 5 2 -3 5 3 2 3 1 -1 9 1	28.17 28.44 28.48 28.53 28.61
.100 .029 .945 .912	49 4 7 13 1	2 2 0 -2 5 2 -2 5 1 2 3 0 -1 7 1	21.66 22.04 22.52 22.71 22.73	3.110 3.098 3.090 3.076 3.076	2 1 2 1 4	0 9 1 -2 7 3 -1 3 4 -3 7 3 1 5 2	28.68 28.79 28.87 29.01 29.01
.900 .894 .751 .716	2 4 50 30 15	1 5 1 0 7 1 1 7 0 -3 0 2 2 4 0	22.78 22.82 23.70 23.93 24.11	3.064 3.054 3.043 3.030 3.026	1 8 2 1 2	0 5 3 -2 8 2 -3 4 1 -3 4 4 0 8 2	29.12 29.22 29.33 29.46 29.50
3.686 3.678 3.665 3.625 3.616	14 5 30 5 14	-3 1 2 -3 1 3 -2 6 2 -2 5 3 0 6 2	24.12 24.18 24.27 24.54 24.60	3.017 2.976 2.956 2.954 2.923	1 5 5 3 4	-2 8 1 -1 4 4 -1 9 2 -3 6 2 0 10 0	29.59 30.01 30.21 30.23 30.56
3.604 3.601 3.594 3.590	6 2 1 5 2	-1 7 2 -2 6 1 -3 2 3 -1 5 3 1 1 2	24.68 24.70 24.75 24.78 24.78	2.904 2.894 2.893 2.866 2.848	2 1 1 4 4	-3 5 1 0 6 3 -3 5 4 -2 8 3 3 0 0	30.76 30.87 30.88 31.18 31.39
3.569 3.543 3.511 3.471 3.467	51 16 1 9 32	-2 0 4 -2 1 4 1 2 2 -1 8 1 -2 2 4	24.93 25.12 25.35 25.64 25.67	2.846 2.834 2.827 2.817 2.795	3 1 2 3 2	-1 5 4 3 1 0 -1 10 1 -3 1 5 3 2 0	31.41 31.54 31.62 31.74 31.99
3.465 3.461 3.449 3.391 3.375	13 8 1 4	-3 3 3 0 8 1 2 5 0 1 3 2 0 3 3	25.69 25.72 25.81 26.26 26.38	2.779 2.776 2.776 2.776 2.776 2.752	1 2 2 1 1	-3 2 5 2 8 0 -3 7 2 -2 9 1 -2 2 5	32.19 32.21 32.22 32.22 32.51
3.339 3.330 3.325 3.325 3.308	10 3 6 20 3	-2 7 2 -3 0 4 -3 1 1 -1 6 3 -3 1 4	26.67 26.75 26.79 26.79 26.93	2.749 2.734 2.732 2.726 2.718	1 4 6 4 2	-3 6 4 1 7 2 -4 2 4 0 7 3 -3 3 5	32.55 32.73 32.75 32.83 32.93
3.307 3.291 3.280 3.262 3.258	1 5 2 3 8	-3 4 3 -2 7 1 2 1 1 -3 2 1 -1 0 4	26.94 27.07 27.17 27.32 27.35	2.713 2.706 2.705 2.699 2.674	1 6 2 6 1	-2 7 4 -4 3 3 -1 10 2 0 0 4 -4 3 4	32.99 33.08 33.09 33.17 33.48

Imipramine Hydrochloride, $C_{19}H_{25}ClN_2$ - (continued)

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
2.657	4	-2 9 3	33.70
2.654	9	0 2 4	33.75
2.653	1	3 4 0	33.75
2.639	1	-3 4 5	33.94
2.630	3	-4 2 2	34.07
2.618	3	2 0 2	34.23
2.617	1	-2 4 5	34.24
2.603	3	-3 7 4	34.42
2.602	2	-3 8 3	34.43
2.601	1	0 3 4	34.46
2.599 2.580 2.577 2.552 2.547	2 2 1 1	-4 4 4 0 11 1 2 2 2 2 1 10 1 -3 5 5	34.48 34.74 34.79 35.14 35.20
2.537	2	1 11 0	35.35
2.531	3	0 4 4	35.43
2.527	1	-2 5 5	35.50
2.511	2	-4 5 4	35.73
2.498	1	-4 3 5	35.92
2.490	1	-1 11 2	36.04
2.478	1	1 5 3	36.22
2.458	1	3 6 0	36.52
2.438	1	-4 6 3	36.83
2.431	2	-4 5 2	36.95
2.416	1	1 9 2	37.18
2.411	1	0 9 3	37.27
2.386	2	1 6 3	37.67
2.384	1	-1 4 5	37.71
2.379	5	-2 11 1	37.78
2.361	6	0 6 4	38.09
2.353	3	3 7 0	38.22
2.344	2	-4 6 2	38.38
2.325	2	-3 9 4	38.70
2.325	2	3 3 1	38.70
2.315 2.311 2.306 2.300 2.296	1 1 1 2	2 9 1 -3 3 6 2 6 2 -1 9 4 -4 4 1	38.87 38.93 39.03 39.13 39.21
2.283	1	-4 6 5	39.44
2.273	1	1 10 2	39.61
2.262	1	-3 4 6	39.81
2.260	2	-5 0 4	39.86
2.248	1	-4 3 6	40.08
2.246	1	3 8 0	40.11
2.233	2	-5 2 4	40.35
2.215	2	3 5 1	40.70
2.204	4	-1 13 1	40.92
2.201	2	0 13 1	40.97

0			
d(A)	I	hkl	2Θ(°) 。
			λ - 1.540598A
2.199	1	-5 2 5	41.00
2.176	2	-1 10 4	41.47
2.175	2	- 5 2 3	41.49
2.169	1	1 2 4	41.60
2.140	î	1 3 4	42.20
2.140	•	1 3 4	72.20
2.138	1	-3 6 6	42.24
2.136	3	4 0 0	42.28
2.134	2	- 3 9 5	42.32
2.122	3	- 2 9 5	42.58
2.120	3	-2 5 6	42.62
0.106		5 0 6	(0.01
2.106	1	-5 0 6	42.91
2.093	2	-4 7 1	43.20
2.088	1	0 14 0	43.30
2.085	2	-5 2 6	43.37
2.085	5	- 2 13 2	43.37
2.077	2	-3 11 4	43.54
2.077	1	3 7 1	43.54
2.073	3	- 2 13 1	43.64
2.064	2	-4 9 2	43.83
2.058	1	-5 1 2	43.95
2.030	•	J 1 2	43.73
2.050	3	-5 6 4	44.14
2.043	2	- 5 2 2	44.30
2.022	2	-4 9 5	44.78
2.022	1	- 4 7 6	44.80
2.013	2	-4 2 7	45.00
2.012	1	-2 12 4	45.02
	1	3 3 2	45.63
1.987	2	4 6 0	46.38
1.956			
1.955	1		46.42
1.946	1	- 5 7 3	46.64
1.945	1	-3 4 7	46.66
1.943	1	3 11 0	46.72
1.937	1	-3 11 5	46.86
1.924	1	- 3 13 2	47.21
1.922	1	- 5 2 7	47.25
1 010	,	0.15	47.07
1.918	1	0 15 1	47.37
1.907	1	0 13 3	47.66
1.897	1	-1 14 3	47.90

Synonyms 1. (-)-7,8-Didehydro-4,5-α-epoxy-17- methylmorphinan-3,6-α-diol hydrochloride hydrate
2. Morphine Chlorhydrate 3. Morphine Chloride Hydrate
Structure Orthorhombic, $P2_12_12_1$ (19), $Z = 4$. The structure was determined by Gylbert [1973].
Atom positions All atoms were in general positions 4(a). Bond lengths were calculated and indicated that the "z" coordinate of atom C3 should be 0.0935. That value was used in these calculations.
Lattice constants a = 13.020(7) A b = 20.751(10) c = 6.941(4)
a/b = 0.6274 c/b = 0.3345
(published values: a = 13.019(7) Å, b = 20.750(10), c = 6.941(4) [Gylbert, 1973]
Volume 1875.3 Å ³
Density (calculated) 1.331 g/cm ³ (measured) 1.310 g/cm ³ [Gylbert, 1973]
Thermal parameters Isotropic. For the hydrogen atoms, overall B = 3.0 [Gylbert, 1973]. For other atoms, isotropic B, were estimated from β_{ij} for individual atoms.
Scattering factors C ⁰ , H ⁰ , Cl ⁰ , N ⁰ , O ⁰ [International Tables, 1962]
Scale factors (integrated intensities) $\gamma = 0.4275 \times 10^{-3}$ I/I (calculated) = 0.421, for reflection with hk ℓ = 020.
Additional patterns 1. PDF card 10-798 [Barnes and Lindsey, 1955]
References Barnes, W. H. and Lindsey, J. M. (1955). Can. J. Chem. 33, 565. Gylbert, L. (1973). Acta Crystallogr. B29, 1630. International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

	alculated	Pattern	(Pea	k he	ights)
d(A)	I		hkl	λ	20(°) ° - 1.540598A
11.02 10.37 8.11 6.11 5.870	6 89 40 100 29	1 0 1 1	1 2 2 0 1	0 0 0 1+ 1	8.02 8.52 10.90 14.48 15.08
5.764 5.273 5.187 4.897 4.818	84 24 17 20 18	0 1 0 0	2 2 4 3 4	1 1 0 1	15.36 16.80 17.08 18.10 18.40
4.746 4.624 4.586 4.316 4.153	35 11 6 15 15	2 2 1 2 0	0 1 3 2 4	1+ 1 1 1	18.68 19.18 19.34 20.56 21.38
4.055 3.955 3.914 3.675 3.622	9 82 26 6 12	2 1 2 3 3	4 4 3 3 1	0 1 1 0 1	21.90 22.46 22.70 24.20 24.56
3.559 3.501 3.469 3.422 3.351	2 32 16 29 7	0 2 0 0	5 4 0 1 0	1 1+ 2+ 2	25.00 25.42 25.66 26.02 26.58
3.329 3.293 3.191 3.123 3.104	7 3 14 33 15	3 0 1 2 0	4 2 2 5 3	0 2 2 1 2+	26.76 27.06 27.94 28.56 28.74
3.054 3.012 3.002 2.938 2.884	3 16 15 13 5	2 1 3 2 0	6 3 5 2 4	0 2+ 0 2+ 2	29.22 29.64 29.74 30.40 30.98
2.833 2.800 2.753 2.727 2.711	1 9 9 2 2	4 2 3 0 3	2 3 5 7 0	1 2 1 1 2	31.56 31.94 32.50 32.82 33.02
2.688 2.668 2.636 2.623 2.608	3 4 2 2 3	3 1 2 3 1	1 7 4 2 5	2 1+ 2 2 2	33.30 33.56 33.98 34.16 34.36
2.560 2.514 2.464 2.448 2.421	12 4	4 2 2 3 5	5 7 5 7 1	0 1+ 2 0+ 1	35.02 35.68 36.44 36.68 37.10

d(A)	I		2Θ(°) .540598A
2.403 2.389 2.373 2.359 2.314	7 3 4 4 2	1 8 1 5 2 1 4 1 2	37.40 37.62 37.88 38.12 38.88
2.299 2.293 2.270 2.244 2.226	3 4 8 6 7	2 6 2 3 5 2 4 6 1+	39.16 39.26 39.68 40.16 40.50
2.221 2.207 2.193 2.188 2.163	6 2 2 2 8	5 4 1 0 3 3 0 9 1	40.58 40.86 41.12 41.22 41.72
2.133 2.121 2.102 2.085 2.080	3 1 2 4 4	3 8 1 5 5 1 1 4 3+	42.34 42.60 43.00 43.36 43.48
2.074 2.061 2.041 2.032 2.010	4 5 1 4 2	6 1 1 3 0 3 3 1 3+	43.60 43.90 44.34 44.56 45.08
2.000 1.996 1.965 1.958 1.947	6 4 1 3 1	5 6 1 1 10 1 4 6 2+	45.30 45.40 46.16 46.34 46.60
1.933 1.923 1.902 1.883 1.873	3 2 2 1 2	6 4 1+ 1 6 3+ 5 7 1+	46.98 47.22 47.78 48.30 48.56
1.867 1.862 1.853 1.844 1.838	4 5 2 1 2	5 5 2 4 7 2+ 2 6 3	48.74 48.88 49.12 49.38 49.56
1.832 1.807 1.803 1.790 1.785	2 2 2 1 1	3 10 1+ 1 11 1 7 1 1	49.72 50.46 50.58 50.98 51.14
1.777 1.765 1.757 1.729 1.726	2 1 1 2 2	1 10 2 3 9 2+ 5 0 3+	51.38 51.76 52.02 52.90 53.00

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		Calculated	Patte	ern	(In	tegrated)
10.38 100 0 2 0 8.52 8.11 46 1 2 0 10.89 6.21 4 2 1 0 14.25 6.12 66 1 0 1 14.25 6.11 59 1 3 0 14.49 5.874 28 1 1 1 15.07 5.769 98 0 2 1 15.35 5.275 28 1 2 1 16.80 5.188 18 0 4 0 17.08 4.900 23 0 3 1 18.09 4.819 19 1 4 0 18.39 4.748 33 2 0 1 18.67 4.741 9 2 3 0 18.70 4.586 5 1 3 1 19.16 4.586 5 1 3 1 19.34 4.318 18 2 2	d(Å)	I		hk	2	
8.11 46 1 2 0 10.89 6.21 4 2 1 0 14.25 6.12 66 1 0 1 14.45 6.11 59 1 3 0 14.49 5.874 28 1 1 1 15.07 5.769 98 0 2 1 15.35 5.275 28 1 2 1 16.80 5.188 18 0 4 0 17.08 4.900 23 0 3 1 18.09 4.819 19 1 4 0 18.39 4.748 33 2 0 1 18.67 4.741 9 2 3 0 18.70 4.629 12 2 1 1 19.16 4.586 5 1 3 1 19.16 4.586 5 1 3 1 19.16 4.586 5 1 3 1	11.03	5	1	1	0	8.01
6.21	10.38	100	0	2	0	8.52
6.12 66 1 0 1 14.45 6.11 59 1 3 0 14.49 5.874 28 1 1 1 1 15.07 5.769 98 0 2 1 15.35 5.275 28 1 2 1 16.80 5.188 18 0 4 0 17.08 4.900 23 0 3 1 18.09 4.819 19 1 4 0 18.39 4.741 9 2 3 0 18.70 4.629 12 2 1 1 19.16 4.586 5 1 3 1 19.34 4.318 18 2 2 1 20.55 4.155 18 0 4 1 21.37 4.057 10 2 4 0 21.89 3.959 86 1 4 1 22.44 3.954 18 1 5 0 22.47 3.915 26 2 3 1 22.70 3.680 1 3 0 1 24.17 3.676 7 3 3 0 2 4.19 3.623 15 3 1 1 24.55 3.562 1 0 5 1 24.98 3.503 30 2 4 1 25.41 3.500 11 2 5 0 25.43 3.470 10 0 0 2 2 25.65 3.468 6 3 2 1 25.67 3.458 1 0 6 0 25.74 3.436 7 1 5 1 25.91 3.423 34 0 1 2 26.91 3.291 3 0 2 2 2 7.07 3.216 3 3 4 0 26.76 3.329 6 3 4 0 26.76 3.310 2 1 2 26.91 3.291 3 0 2 2 2 7.07 3.216 3 4 1 0 27.72 3.191 18 1 2 2 7.94 3.125 43 2 5 1 28.54 3.106 5 4 2 0 28.72 3.102 10 0 3 2 28.76 3.054 2 2 6 0 29.22 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 4 1 29.74 3.001 2 3 5 0 29.76	8.11	46	1	2	0	10.89
6.11	6.21	4	2	1	0	14.25
5.874 28 1 1 1 15.07 5.769 98 0 2 1 15.35 5.275 28 1 2 1 16.80 5.188 18 0 4 0 17.08 4.900 23 0 3 1 18.09 4.819 19 1 4 0 18.39 4.741 9 2 3 0 18.67 4.741 9 2 3 0 18.70 4.629 12 2 1 1 19.16 4.586 5 1 3 1 19.34 4.318 18 2 2 1 20.55 4.155 18 0 4 1 21.37 4.057 10 2 4 0 21.89 3.959 86 1 4 1 22.44 3.915 26 2 3 1 22.70 3.680 1 3 0	6.12	66	1	0	1	14.45
5.874 28 1 1 1 15.07 5.769 98 0 2 1 15.35 5.275 28 1 2 1 16.80 5.188 18 0 4 0 17.08 4.900 23 0 3 1 18.09 4.819 19 1 4 0 18.39 4.741 9 2 3 0 18.70 4.629 12 2 1 1 19.16 4.586 5 1 3 1 19.34 4.318 18 2 2 1 20.55 4.155 18 0 4 1 21.37 4.057 10 2 4 0 21.89 3.959 86 1 4 1 22.44 3.915 26 2 3 1 22.70 3.680 1 3 0 1 24.17 3.676 7 3 3	6.11	59	1	3	0	14.49
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	2.947	5				30.30

d(A)	Ι		hkl	2Θ(°) 。 λ - 1.540598A
2.945 2.937 2.918 2.890 2.885	3 12 2 1 6	4 2 4 1 0	2 1 7	0 30.32 2 30.41 1 30.62 0 30.91 2 30.98
2.835 2.816 2.800 2.757 2.753	1 3 11 1	4 1 2 4 3	3 2 4	1 31.53 2 31.75 2 31.93 0 32.45 1 32.49
2.726 2.710 2.698 2.688 2.668	2 2 1 3 5	0 3 2 3 1	0 2 7 1	1 32.83 2 33.02 0 33.18 2 33.31 1 33.56
2.662 2.637 2.622 2.608 2.561	1 2 3 3 3	0 2 3 1 4	4 2 2 3 5 3	2 33.64 2 33.97 2 34.16 2 34.35 0 35.01
2.524 2.520 2.515 2.464 2.450	5 6 10 5 2	3 3 2 2 0	6 7 5	2 35.54 1 35.60 1 35.68 2 36.43 2 36.65
2.448 2.421 2.403 2.402 2.389	5 7 3 6 3	3 5 4 3 1	1 5 4	0 36.68 1 37.10 1 37.40 2 37.40 1 37.63
2.373 2.359 2.314 2.299 2.293	5 5 3 3 3	5 4 4 5 2	1 2 2 3	1 37.88 2 38.12 2 38.88 1 39.14 2 39.26
2.276 2.269 2.246 2.243 2.227	1 11 3 6 7	2 3 4 4 3	5 : 3 : 6	1 39.56 2 39.68 2 40.12 1 40.17 0 40.48
2.225 2.221 2.207 2.194 2.188	1 3 2 1 1	1 1 5 0 0	7 3 4 3 3	3 40.51 2 40.59 1 40.86 3 41.11 1 41.22
2.173 2.168 2.164 2.133 2.133	1 5 8 1 3	2 2 1 2 3	1 3 2	0 41.52 3 41.62 3 41.71 3 42.33 2 42.33
	2.945 2.937 2.918 2.890 2.885 2.835 2.816 2.800 2.757 2.753 2.726 2.710 2.698 2.688 2.668 2.662 2.637 2.622 2.608 2.561 2.524 2.520 2.515 2.464 2.450 2.448 2.421 2.403 2.402 2.389 2.373 2.359 2.314 2.299 2.293 2.276 2.269 2.246 2.243 2.277 2.225 2.246 2.243 2.277 2.194 2.188 2.173 2.168 2.168 2.173 2.168 2.173 2.168 2.173 2.168 2.173 2.168 2.173 2.168 2.173 2.168 2.173 2.168 2.164 2.133	d(A) I 2.945 3 2.937 12 2.918 2 2.890 1 2.885 6 2.835 1 2.816 3 2.800 11 2.757 1 2.753 11 2.726 2 2.710 2 2.698 1 2.688 3 2.662 1 2.637 2 2.622 3 2.608 3 2.561 3 2.524 5 2.520 6 2.515 10 2.4644 5 2.4450 2 2.448 5 2.421 7 2.403 3 2.373 5 2.314 3 2.299 3 2.227 7 2.225 1 2.221 3 2.269 1 2.225	d(A) I 2.945 3 4 2.937 12 2 2.918 2 4 2.890 1 1 2.885 6 0 2.835 1 4 2.816 3 1 2.800 11 2 2.757 1 4 2.726 2 0 2.710 2 3 2.698 1 2 2.688 3 3 2.662 1 0 2.637 2 2 2.608 3 1 2.524 5 3 2.551 10 2 2.464 5 2 2.450 2 3 2.450 2 3 2.373 5 5 2.373 5 5 2.389 3 1 2.269 11 3 2.269 11 3 2.246 3	d(A) I hkl 2.945 3 4 3 2.937 12 2 2 2.918 2 4 1 2.890 1 1 7 2.885 6 0 4 2.835 1 4 2 2.816 3 1 4 2.800 11 2 3 2.757 1 4 4 2.753 11 3 5 2.726 2 0 7 2.698 1 2 7 2.688 3 3 1 2.668 5 1 7 2.662 1 0 5 2.637 2 2 4 2.608 3 1 5 2.524 5 3 3 2.520 6 3 6 2.515 10 2 7 2.464 5 2 5 2.470 2

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
2.120 2.102 2.090 2.086 2.083	1 3 1 3 1	3 8 1 5 5 1 4 7 1 1 4 3 5 0 2	42.61 42.99 43.25 43.35 43.41
2.079 2.074 2.061 2.061 2.042	1 2 6 1	2 3 3 2 9 1 6 1 1 4 5 2 3 0 3	43.49 43.60 43.90 43.90 44.33
2.032 2.031 2.029 2.021 2.010	3 2 1 1 2	3 1 3 6 2 1 4 8 0 0 5 3 2 4 3	44.56 44.58 44.63 44.81 45.07
2.003 2.000 1.993 1.965 1.958	1 6 1 1	3 2 3 3 7 2 5 6 1 1 10 1 3 3 3	45.23 45.30 45.48 46.15 46.33
1.957 1.947 1.933 1.930 1.924	2 1 3 1	4 6 2 4 8 1 5 4 2 2 5 3 6 4 1	46.35 46.61 46.97 47.05 47.21
1.923 1.902 1.883 1.874 1.867	1 2 1 2 4	0 6 3 1 6 3 5 7 1 3 8 2 1 11 0	47.23 47.77 48.29 48.54 48.74
1.862 1.853 1.844 1.838 1.832	4 1 1 1	5 5 2 4 7 2 2 6 3 5 8 0 3 5 3	48.89 49.12 49.38 49.56 49.73
1.812 1.808 1.803 1.790 1.784	1 2 1 1	2 11 0 3 10 1 1 11 1 7 1 1 5 6 2	50.32 50.45 50.59 50.98 51.15
1.777 1.765 1.756 1.730 1.727	1 1 1 1 2	5 8 1 1 10 2 3 9 2 5 0 3 0 8 3	51.39 51.77 52.03 52.89 52.99

Synonyms	Calc	culated Pat	ttern	(Pea	k he	ights)
1. 17-Allyl-4,5-epoxy-3,14-dihydroxy- morphinan-6-one hydrochloride hydrate 2. (-)-N-Allyl-7,8-dihydro-14-hydroxy-	d(Å)	I		hkl		20(°) - 1.540598A
morphinone hydrochloride hydrate Structure	10.75 9.28	6 2	0		1 2	8.22 9.52
Orthorhombic, $P2_12_12_1$ (19), $Z = 4$. The structure was refined in 1975 by Sime et al., and in 1974 by Karle.	7.58 7.21 6.73	13 100 11	0	1 0 1	2	11.66 12.26 13.14
Atom positions All atoms were in the general positions 4(a) given by Sime et al. [1975]. The "x" parameter for C(15) appeared to be in error, and the value 0.1908 was used instead, in these calculations.	6.59 6.33 5.45 5.37 4.87	27 26 27 6 12	1 0	1 1 2	2	13.42 13.98 16.26 16.48 18.22
Lattice constants	4.55	5		1		19.48
$a = 7.833(3) \stackrel{\circ}{A}$ b = 13.186(5) c = 18.570(5)	4.51 4.43 4.28	2 11 2	1 0	2 2 3	2	19.66 20.02 20.76
0	3.911	5	1	2	3+	22.72
(published values: a = 7.833(3) A, b = 13.185(5), c = 18.569(5) [Sime et al.,1975])	3.831 3.751 3.678	11 23 3	1	3 3 1		23.20 23.70 24.18
CD cell: a = 13.185(5), b = 18.570(5), c = 7.833(3); sp. gp. = P2 ₁ 2 ₁ 2 ₁ ; a/b = 0.7101, c/b = 0.4218	3.607 3.542	6 11	2	0	2 2	24.66 25.12
Volume	3.480 3.414 3.356	4 2 7	1 1	1 2 0	4 5+	25.58 26.08 26.54
Density (calculated) 1.385 g/cm ³ (measured) 1.35 g/cm ³ [Sime et al.]	3.312 3.252	18 5	1	3	1 3+	26.90 27.40
(measured) 1.35 g/cm [bline et al.]	3.209 3.164	2 1		1 2		27.78 28.18
Thermal parameters Isotropic. For hydrogen: overall B = 4.0	3.038	10	1	4	0	29.38
and for other atoms, B. was estimated from B.; for individual atoms.	2.992 2.955	9 6		2	5+ 4+	29.84 30.22
Scattering factors	2.917	3		1	4+	30.62
H ^O [International Tables, 1962]	2.912	3 3	0	4	3	30.68 30.94
All other atoms, zero ionization, from Cromer	2.790	6	2	3	2	32.06
and Mann [1968]. The chlorine atoms were corrected for dispersion [Cromer and Liberman, 1970].	2.727	4	2	2	4+	32.82
Carla fratium (imbarustal imbaruitian)	2.687	2	0	4	4	33.32
Scale factors (integrated intensities) $\gamma = 1.196 \times 10^{-3}$	2.667	1		3		33.58
I/I corundum (calculated) = 1.13 for the	2.638	6 2		2		33.96 35.02
reflection with hkl = 101.	2.542	1	1	4	4+	35.28
References	2.521	1	2	4	0	35.58
Cromer, D. T. and Mann, J. B. (1968). Acta	2.498	4		4		33.92
Crystallogr. A24, 321.	2.468	5		1		36.38
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.	2.426 2.408	2 2	0 1	5 3	3+ 6+	37.02 37.32
International Tables for X-ray Crystallography,						
III (1962). (The Kynoch Press, Birmingham,	2.348	4		2	7+ 6	38.30
Eng.), p. 202.	2.278	2 2		2 4	6 6+	39.52 39.92
Karle, I. L. (1974). Acta Crystallogr. <u>B30</u> , 1682.	2.257	1	1		8	40.50
Sime, R. L., Forehand, R. and Sime, R. J. (1975).	2.201	2	1		4	40.98

Acta Crystallogr. B31, 2326.

Naloxone Hydrochloride Hydrate, $C_{19}H_{22}C1NO_4 \cdot 2H_2O$ - (continued)

d(A)	Ι	hkl 20(°) ο λ - 1.540598A
2.182	2	3 3 2+ 41.34
2.173	1	2 5 1 41.52
2.151	1	3 2 4 41.96
2.129	2	2 5 2 42.42 3 3 3+ 42.82
2.110	2	3 3 3+ 42.82
2.086	1	2 4 5+ 43.34
2.063	2	1 6 2+ 43.86
2.047	1	3 4 0 44.22
1.999	3	3 4 2+ 45.34
1.973	1	3 1 6+ 45.96
1.944	1	1 5 6+ 46.68
1.921	1	3 3 5+ 47.28
1.910	2	1 2 9+ 47.58
1.896	1	4 1 2 47.94
1.892	1	4 1 2 47.94 0 6 5 48.06
1.868	1	0 3 9+ 48.72
1.855	1	3 5 0 49.06
1.839	2	4 2 2+ 49.52

	Calculated	Pattern	(Inte	egrated)
d(A)	I	hks		20(°) \ - 1.540598Å
10.75 10.75 9.28 9.28 7.59 7.59 7.22 7.22 6.73 6.73 6.59 6.33 6.33 5.45 5.45 5.38 4.87 4.87 4.56 4.56 4.51	6 6 2 2 12 100 100 9 9 27 27 26 27 28 28 4 4 13 12	0 1 0 -1 0 0 0 0 0 1 0 -1 1 0 -1 0 1 1 -1 -1 0 2 0 -2 1 1 -1 -1 1 1 -1 -1 1 2 0 2 0 -2 1 1 1 -1 -1 1 1 0 2 0 -2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1	1 -1 2 -2 2 -2 1 -1 0 0 0 1 -1 2 -2 2 -2	8.22 8.22 9.52 9.52 11.65 11.65 12.25 12.25 13.14 13.14 13.42 13.42 13.98 13.98 16.25 16.25 16.48 16.48 16.48 18.21 19.46 19.46 19.66
4.51 4.43	1 12	0 -2 1 2	-3 2	19.66 20.02

0		
d(Å)	I	hkl 2Θ(°) ° λ - 1.540598A
4.43	11	-1 -2 -2 20.02
4.28	2	0 3 1 20.75
4.28	2	0 -3 -1 20.75
3.916	3	2 0 0 22.69
3.916	3	-2 0 0 22.69
3.910	3	1 2 3 22.72
3.910	3	-1 -2 -3 22.72
3.833	11	1 3 0 23.19
3.833	11	-1 -3 0 23.19
3.822	2	1 1 4 23.25
3.822	1	-1 -1 -4 23.25
3.754	11	2 1 0 23.68
3.754	11	-2 -1 0 23.68
3.754	14	1 3 1 23.68
3.754	15	-1 -3 -1 23.68
3.680	3	2 1 1 24.17
3.680	3	-2 -1 -1 24.17
3.609	6	2 0 2 24.65
3.609	6	-2 0 -2 24.65
3.543	12	1 3 2 25.11
3.543	12	-1 -3 -2 25.11
3.481	4	2 1 2 25.57
3.481	4	-2 -1 -2 25.57
3.416	2	1 2 4 26.07
3.416	2	-1 -2 -4 26.07
3.367	3	2 2 0 26.45
3.367	3	-2 -2 0 26.45
3.356	5	1 0 5 26.54
3.356	5	-1 0 -5 26.54
3.313	19	2 2 1 26.89
3.313	18	-2 -2 -1 26.89
3.310	2	2 0 3 26.92
3.310	2	-2 0 -3 26.92
3.259	3	1 3 3 27.34
3.259	3	-1 -3 -3 27.34
3.252 3.252 3.246 3.246 3.236	3 3 1 1	1 1 5 27.40 -1 -1 -5 27.40 0 4 1 27.46 0 -4 -1 27.46 0 2 5 27.54
3.236	1	0 -2 -5 27.54
3.210	2	2 1 3 27.77
3.210	2	-2 -1 -3 27.77
3.165	1	2 2 2 28.17
3.165	1	-2 -2 -2 28.17
3.038 3.038 2.994 2.994 2.991	12 12 4 4 6	1 4 0 29.37 -1 -4 0 29.37 2 0 4 29.82 -2 0 -4 29.82 1 2 5 29.85
	•	

d(A)	Ι	hkl	2Θ(°) ° λ - 1.540598A
2.991	6	-1 -2 -5	29.85
2.958	3	2 2 3	30.19
2.958	3	-2 -2 -3	30.19
2.956	4	1 3 4	30.21
2.956	4	-1 -3 -4	30.21
2.924	1	2 3 0	30.55
2.924	1	-2 -3 0	30.55
2.919	2	2 1 4	30.60
2.919	2	-2 -1 -4	30.60
2.910	2	0 4 3	30.70
2.910	2	0 -4 -3	30.70
2.888	2	1 4 2	30.94
2.888	2	-1 -4 -2	30.94
2.812	1	1 1 6	31.79
2.812	1	-1 -1 -6	31.79
2.802	2	0 2 6	31.92
2.802	2	0 -2 -6	31.92
2.789	7	2 3 2	32.07
2.789	7	-2 -3 -2	32.07
2.728	2	1 4 3	32.81
2.728	2	-1 -4 -3	32.81
2.726	3	2 2 4	32.83
2.726	3	-2 -2 -4	32.83
2.688	2	0 4 4	33.31
2.688	2	0 -4 -4	33.31
2.667 2.667 2.644 2.644 2.640	1 1 1 1	1 3 5 -1 -3 -5 2 3 3 -2 -3 -3 2 1 5	33.57 33.57 33.88 33.88 33.92
2.640	1	-2 -1 -5	33.92
2.638	6	1 2 6	33.96
2.638	6	-1 -2 -6	33.96
2.561	2	3 1 0	35.01
2.561	2	-3 -1 0	35.01
2.542	1	1 4 4	35.27
2.542	1	-1 -4 -4	35.27
2.522	1	2 4 0	35.57
2.522	1	-2 -4 0	35.57
2.499	4	2 4 1	35.91
2.499	4	-2 -4 -1	35.91
2.474	1	2 3 4	36.28
2.474	1	-2 -3 -4	36.28
2.469	3	3 1 2	36.36
2.469	3	-3 -1 -2	36.36
2.465 2.465 2.428 2.428 2.426	2 2 1 1	0 4 5 0 -4 -5 3 2 0 -3 -2 0 0 5 3	36.41 36.41 37.00 37.00 37.02

d(Å)	I	hkl	2Θ(°) λ - 1.540598A
2.426	1	0 -5 -3	37.02
2.408	1	1 3 6	37.31
2.408	1	-1 -3 -6	37.31
2.349	2	3 2 2	38.29
2.349	2	-3 -2 -2	38.29
2.348	3	1 2 7	38.30
2.348	3	-1 -2 -7	38.30
2.279	2	2 2 6	39.52
2.279	2	-2 -2 -6	39.52
2.256	2	0 4 6	39.92
2.256	2	0 -4 -6	39.92
2.226	1	1 0 8	40.50
2.226	1	-1 0 -8	40.50
2.201	2	1 5 4	40.98
2.201	2	-1 -5 -4	40.98
2.182 2.182 2.172 2.172 2.151	1 1 1 1	3 3 2 -3 -3 -2 2 5 1 -2 -5 -1 3 2 4	41.35 41.35 41.53 41.53 41.96
2.151	1	-3 -2 -4	41.96
2.129	2	2 5 2	42.42
2.129	2	-2 -5 -2	42.42
2.110	2	3 3 3	42.82
2.110	2	-3 -3 -3	42.82
2.086 2.086 2.063 2.063 2.047	1 1 1 1	2 4 5 -2 -4 -5 1 6 2 -1 -6 -2 3 4 0	43.33 43.33 43.85 43.85 44.22
2.047	1	-3 -4 0	44.22
1.999	2	3 4 2	45.34
1.999	2	-3 -4 -2	45.34
1.944	1	1 5 6	46.67
1.944	1	-1 -5 -6	46.67
1.910 1.910 1.896 1.896 1.891	1 1 1 1	1 2 9 -1 -2 -9 4 1 2 -4 -1 -2 0 6 5	47.58 47.58 47.94 47.94 48.07
1.891 1.840 1.840 1.839 1.839	1 1 1 1	0 -6 -5 4 2 2 -4 -2 -2 0 1 10 0 -1-10	48.07 49.50 49.50 49.53 49.53

Structure Cubic, Z = 2. The space group Pm3m was used for the structure determination by Geller [1962] and for the powder pattern here. The x-ray data did not eliminate uncertainty about the space group which could also be P43m or P432 [Geller, 1962]. Atom positions 24(m) 24 palladium 12(j) 12 selenium 12 selenium 12(i) 6 selenium 6(f) 6(e) 6 palladium 3(d) 3 palladium 1(b) 1 palladium

Lattice constants a = 10.607(3) A

(published value: $a = 10.606(3) \stackrel{\circ}{A}$ [Geller, 1962]).

Volume o 1193.4 A³

Density (calculated) 8.330 g/cm³

Thermal parameters
Isotropic, Table 2 [Geller, 1962]

Scattering factors

Pd⁰, Se⁰ [Thomas and Umeda, 1957], corrected for dispersion [Cromer and Liberman, 1970]

Scale factor (integrated intensities) $\gamma = 0.4090 \times 10^{-3}$ I/I corundum (calculated) = 4.11 for reflection with hkl = 440.

References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. <u>53</u>, 1891. Geller, S. (1962). Acta Crystallogr. <u>15</u>, 713. Thomas, L. H. and Umeda, K. (1957). J. Chem. Phys. <u>26</u>, 293.

Calc	culated Pat	tern (Pea	ak heights)	
d(Å)	I	hkl	2Θ(°) λ - 1.540598	o A
5.30	5	2 0	0 16.72	
4.741	3	2 1	0 18.70	
4.329	1	2 1	1 20.50	
3.748	4	2 2	0 23.72	
3.534	4	2 2	1 25.18	
3.353	44	3 1	0 26.56	
3.198	91	3 1	1 27.88	
3.062	3	2 2	2 29.14	
2.942	18	3 2	0 30.36	
2.834	52	3 2	1 31.54	
2.572	64	4 1	0+ 34.86	
2.499	32	4 1	1 35.90	
2.4327	26	3 3	1 36.92	
2.3720	25	4 2	0 37.90	
2.3145	20	4 2	1 38.88	
2.1215 2.0797 2.0413 1.9365 1.8748	11 12 79 1	4 3 4 3 3 3 5 2 4 4	0+ 42.58 1+ 43.48 3 44.34 1 46.88 0 48.52	
1.8462	3	5 2	2 49.32	
1.8193	9	4 3	3+ 50.10	
1.7925	1	5 3	1 50.90	
1.7679	36	6 0	0 51.66	
1.7435	4	6 1	0 52.44	
1.7203	16	5 3	2+ 53.20	
1.6772	6	6 2	0 54.68	
1.6566	17	5 4	0+ 55.42	
1.6365	15	5 4	1 56.16	
1.6175	3	5 3	3 56.88	
1.5814	5	5 4	2+ 58.30	
1.5309	2	4 4	4 60.42	
1.5155	2	7 0	0 61.10	
1.5000	5	7 1	0+ 61.80	
1.4853	1	5 5	1 62.48	
1.4709	5	6 4	0 63.16	
1.4569	2	6 4	1 63.84	
1.4049	2	5 4	4+ 66.50	
1.3927	3	7 3	0 67.16	
1.3807	25	7 3	1 67.82	
1.3579	5	6 4	3 69.12	
1.3470	6	7 3	2+ 69.76	
1.3258	9	8 0	0 71.04	
1.3156	3	7 4	0+ 71.68	
1.3055	9	5 5	4+ 72.32	
1.2959 1.2862 1.2770 1.2677 1.2501	12 12 5 . 1	7 3 6 4 7 4 6 5 6 6	3 72.94 4 73.58 2+ 74.20 3 74.84 0 76.08	

Palladium Selenium (Palladseite), $Pd_{17}Se_{15}$ - (continued)

d(Å)	I	hkl 20(°) ° λ - 1.540598Å
1.2415	1	8 3 0+ 76.70
1.2331	6	7 4 3 77.32
1.2248	5	7 5 1 77.94
1.2167	1	6 6 2 78.56
1.1858	3	8 4 0 81.02
1.1786	3	7 4 4+ 81.62
1.1713	4	9 1 0 82.24
1.1643	1	9 1 1+ 82.84
1.1573	5	8 4 2 83.46
1.1505	3	7 6 0 84.06
1.1437	7	7 6 1+ 84.68

	Calculated	Patt	ern	(In	tegrated)
d(Å)	I		hk	2	2Θ(°) λ - 1.540598A
5.30 4.744 4.330 3.750 3.536	4 2 1 3 3	2 2 2 2 2	0 1 1 2 2	0 0 1 0	16.70 18.69 20.49 23.71 25.17
3.354 3.198 3.062 2.942 2.835	38 79 3 16 47	3 3 2 3 3	1 1 2 2	0 1 2 0 1	26.55 27.87 29.14 30.36 31.53
2.573 2.573 2.500 2.4334 2.3718	44 16 29 24 23	4 3 4 3 4	1 2 1 3	0 2 1 1 0	34.85 34.85 35.89 36.91 37.90
2.3146 2.1214 2.1214 2.0802 2.0802	19 5 5 5 6	4 4 5 5 4	0 1	1 0 0 0 1	38.88 42.58 42.58 43.47 43.47
2.0413 2.0413 1.9366 1.8751 1.8464	6 71 1 100 2	5 3 5 4 5	3 2 4	1 3 1 0 2	44.34 44.34 46.88 48.51 49.31
1.8191 1.8191 1.7929 1.7678 1.7438	2 7 1 36 4	5 4 5 6	3 3 0	0 3 1 0 0	50.11 50.11 50.89 51.66 52.43
1.7207 1.7207 1.6771 1.6565 1.6565	6 10 6 7 3	6 5 6 5	3 2 4	0	53.19 53.19 54.68 55.42 55.42

d(A)	I	h	kl		2Θ(°) λ - 1.540598A
1.6565	7	4	4	3	55.42
1.6367	15	5	4	1	56.15
1.6176	3	5	3	3	56.88
1.5812	3	5	4	2	58.31
1.5812	2	6	3	0	58.31
1.5310 1.5153 1.5001 1.5001 1.4853	2 2 3 2	4 7 7 5 5	4 0 1 5 5	4 0 0 0 1	60.42 61.11 61.80 61.80 62.48
1.4709 1.4570 1.4049 1.3928 1.3809	5 2 2 2 2 27	6 6 5 7 7	4 4 4 3 3	0. 1 4 0	63.16 63.83 66.50 67.16 67.81
1.3581 1.3471 1.3471 1.3259 1.3156	5 3 3 10 3	6 7 6 8 7	4 3 5 0 4	3 2 1 0	69.11 69.76 69.76 71.04 71.68
1.3056	3	7	4	1	72.31
1.3056	1	8	1	1	72.31
1.3056	6	5	5	4	72.31
1.2959	13	7	3	3	72.94
1.2863	13	6	4	4	73.58
1.2769	4	7	4	2	74.20
1.2769	1	8	2	1	74.20
1.2678	1	6	5	3	74.83
1.2500	9	6	6	0	76.08
1.2330	6	7	4	3	77.32
1.2248	5	7	5	1	77.94
1.2167	1	6	6	2	78.56
1.1859	3	8	4	0	81.02
1.1786	2	7	4	4	81.63
1.1713	4	9	1	0	82.24
1.1643	1	9	1	1	82.85
1.1573	5	8	4	2	83.46
1.1505	3	7	6	0	84.06
1.1438	4	7	6	1	84.67
1.1438	3	9	2	1	84.67

Synonyms	Calc	culated Pa	ttern	(Pe	ak l	heights)
 1. 1-(1-Phenylcyclohexyl) piperidine hydrochloride 2. Sernyl hydrochloride 3. Sernylan 	d(Å)	I		hkl		2Θ(°) ° λ - 1.540598A
4. PCP hydrochloride	9.34 8.58	16 57	0 1	1 0		9.46 10.30
CAS registry no. 956-90-1	6.93 6.34 6.08	6 15 100	0 0	2 0 2	0 2	12.76 13.96 14.56
Structure Monoclinic, $P2_1/c$ (14), $Z = 4$. The structure was determined by Argos et al. [1970].	5.80 5.76	15 22		1	2	15.26 15.36
Atom positions All atoms were in general positions [ibid.]	5.39 5.27 4.68	2 14 18	-1	1 2 2	1	16.44 16.80 18.96
Lattice constants	4.47	19		2		19.84
a = 8.881(10) A b = 13.867(20)	4.34	22 25	2	0	0	20.44
c = 13.099(10) $\beta = 104.55(16)^{\circ}$	4.10 4.05	9 38		1		21.64 21.92
(published values: a = 8.881(10), b = 13.866(20), c = 13.098(10), β = 104°33'(10') [Argos et al., 1970])	3.90 3.82 3.73 3.65	18 26 11 26	1 -2	1 2 2 1	2	
CD cell: $a = 13.099(10)$ Å, $b = 13.867(20)$,	3.62	23		3		
c = 8.881(10), β = 104.55(16)°; sp. gp. P2 ₁ /a; a/b = 0.9446; c/b = 0.6404	3.36 3.33	2 11	2	1 2	1	26.52 26.78
Volume o 1561.4 A ³	3.25 3.21 3.16	3 3 24	1	3 4 1	0	27.40 27.74 28.18
Density (calculated) 1.190 g/cm ³ (measured) 1.190(4) [Argos et al., 1970]	3.12 3.05 2.942	23 3 4		3 4 2		29.28
Thermal parameters Isotropic B_i , estimated from β_{ij} for individual atoms.	2.895 2.864	9 7		1	1+ 4+	
	2.773 2.722	4 6		3 4	3+ 1+	
Scattering factors Zero ionization [International Tables, 1962]	2.696 2.682	3 5		2 4		
Scale factors (integrated intensities) $\gamma = 0.6975 \times 10^{-3}$	2.624	7	-1	5	1	34.14
I/I_{corundum} (calculated) = 0.751 for reflection with hk ℓ = 021.	2.608 2.541 2.510	4 1 1	2	5 2	3	35.74
Additional pattern 1. Folen [1975]	2.493 2.455	3	-3 -2	3	1+ 3+	
References Argos, P., Barr, R. E., and Weber, A. H. (1970). Acta Crystallogr. <u>B26</u> , 53. Folen, V. A. (1975). J. Forensic Sci. <u>20</u> , 348.	2.368 2.361 2.329 2.277 2.251	2 2 4 2 5		1 2 3	5+	38.08 38.62
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.	2.223 2.180 2.166 2.149	3 2 2 2	-2	6 3 2		41.38 41.66
	2.149	.5	2		3	42.48

1	culated	Pattern	(Pe	ak l	neights)
d(A)	I		hkl		2Θ(°) λ - 1.540598Å
2.123 2.107 2.053 2.026 2.022	5 3 4 4 4	4 -4 4 -2 0	1 2 2 2 2	0+ 1+ 0+ 6+	42.54 42.88 44.08 44.70 44.78
2.015 1.995 1.980 1.948 1.942	5 2 2 2 2	4 -4 -3 4	1 3 3 3 0	1+ 1+ 5 0+ 6	44.96 45.42 45.78 46.58 46.74
1.930 1.926 1.891 1.870 1.846	5 4 2 2 1	1 -1 0 1 -2	7 7 7 2 5	0+ 1+ 2+ 6+ 5+	47.04 47.16 48.08 48.64 49.34
1.818 1.805 1.794 1.762 1.756	1 1 1 1 2	3 -1 0 1 2	4 2 7 5 7	3 7+ 3+ 5+ 1+	50.14 50.52 50.86 51.86 52.04
1.750 1.719 1.700 1.696 1.689	1 1 2 2 2	-4 2 -5 1 -5	3 1 2 4 1	5 6+ 3+ 6+ 4+	52.22 53.24 53.88 54.02 54.28
1.672 1.662 1.646 1.641 1.622	1 1 1 1	0 -1 -1 1 -1	8 8 4 2 1	2 2 7 7+ 8+	54.86 55.22 55.82 56.00 56.70
1.614 1.586 1.563	1 1 1	-5 1 -3	1 3 0	5+ 7+ 8+	57.00 58.10 59.06

Ca	alculated 1	Pattern	(I	nte	grated)
d(A)	I		hkl		2Θ(°) λ - 1.540598Å
9.36	16	0	1	1	9.44
8.60	57	1	0	0	10.28
7.01	1	-1	1	1	12.62
6.93	6	0	2	0	12.76
6.34	14	0	0	2	13.96
6.08	100	0	2	1	14.55
5.85	1	- 1	0	2	15.13
5.82	10	1	1	1	15.22
5.77	19	0	1	2	15.36
5.39	1	-1	1	2	16.43

d(Å)	I	ŀ	nkl		2Θ(°) 。 λ - 1.540598A
5.27 4.71 4.68 4.47 4.35	14 3 17 19 1	-1 1 0 -1 1	2 2 2	1 1 2 2 2	16.80 18.84 18.95 19.84 20.40
4.34 4.30 4.11 4.06 4.05	21 25 7 10 33	0 2 2 -2 -1	0 1 0	1 0 0 2 3	20.43 20.65 21.63 21.86 21.91
4.04 4.02 3.90 3.82 3.75	1 4 19 28 1	0 -1 -2 1 1	3 1 2	3 1 2. 2	21.97 22.11 22.79 23.25 23.72
3.73 3.66 3.65 3.63 3.62	11 16 11 17 9	-2 2 2 -1 -1	1 2 3	1 1 0 2 3	23.85 24.32 24.35 24.52 24.60
3.61 3.36 3.33 3.25 3.22	1 2 12 3 2	0 1 2 1 1	1 2 3	3 3 1 2	24.65 26.50 26.78 27.39 27.72
3.19 3.17 3.17 3.15 3.12	4 7 20 9 9	-1 0 -1 2 2	0 1 3	1 4 4 0 2	27.96 28.13 28.17 28.33 28.58
3.12 3.11 3.05 2.943 2.908	15 3 2 5 2	0 -2 1 -1 2	2 4 2	3 3 1 4 2	28.60 28.66 29.27 30.34 30.72
2.899 2.894 2.865 2.863 2.781	5 5 4 4 2	-3 -3 3 -2 -2	1 0 1	2 1 0 4 3	30.82 30.87 31.19 31.21 32.16
2.772 2.728 2.722 2.709 2.696	3 4 3 2 2	1 -2 -3 0 -2	4 2 5	3 1 1 1 4	32.27 32.80 32.88 33.04 33.20
2.683 2.639 2.637 2.625 2.614	4 2 1 8 1	-1 1 -2 -1 0	5 4 5	3 0 2 1 4	33.37 33.94 33.97 34.13 34.28
2.608 2.541 2.511 2.494 2.492	3 1 1 1 3	3 0 2 0 -3	5 2 1	1 2 3 5 1	34.36 35.30 35.73 35.97 36.01

Phencyclidine Hydrochloride, $C_{17}H_{26}ClN$ - (continued)

d(Å)	I	hkl	2Θ(°) ° λ - 1.540598A
2.457 2.454 2.449 2.368 2.360	2 1 1 1	-2 4 3 -3 0 4 -1 2 5 1 3 4 3 1 2	36.54 36.58 36.67 37.96 38.10
2.337	1	-3 3 3 2 5 0 -2 2 5 -1 5 3 -1 3 5	38.49
2.330	1		38.60
2.329	3		38.63
2.321	1		38.77
2.277	2		39.54
2.260	1	2 1 4	39:85
2.251	5	1 1 5	40.02
2.223	3	-1 6 1	40.55
2.185	1	-4 1 1	41.29
2.180	2	-2 3 5	41.38
2.167	1	1 2 5	41.64
2.165	1	1 5 3	41.69
2.150	1	-1 6 2	42.00
2.149	2	4 0 0	42.01
2.127	5	2 4 3	42.46
2.124	2	4 1 0	42.53
2.121	1	-4 1 3	42.60
2.113	1	0 0 6	42.76
2.108	2	-4 2 1	42.87
2.053	4	4 2 0	44.08
2.053 2.032 2.026 2.024 2.021	1 1 2 1	2 3 4 -4 0 4 -2 2 6 -3 5 1 0 2 6	44.08 44.56 44.69 44.75 44.80
2.015	4	4 1 1	44.96
2.013	2	-2 5 4	45.00
1.996	1	-4 3 1	45.41
1.995	1	-4 3 2	45.43
1.980	3	-3 3 5	45.78
1.949	1	4 3 0	46.57
1.942	1	1 0 6	46.74
1.932	1	2 5 3	46.98
1.930	4	1 7 0	47.04
1.925	1	-1 7 1	47.19
1.893 1.891 1.870 1.867 1.818	1 1 1 1	1 7 1 0 7 2 1 2 6 0 6 4 3 4 3	48.03 48.08 48.65 48.72 50.13
1.805 1.750 1.701 1.700 1.688	1 1 1 1	-1 2 7 -4 3 5 -5 0 4 -5 2 3 -5 1 4	50.52 52.24 53.86 53.88 54.29

d(A)	Ι		hkl	,	2Θ(°) λ - 1.540598Å
1.672	1	0	8	2	54.87
1.662	1	-1	8	2	55.22
1.646	1	-1	4	7	55.82
1.622	1	-1	1	8	56.70
1.586	1	1	3	7	58.10

2Θ(°) - 1.540598A

> 9.98 11.54 12.46 12.98 14.94 16.80 17.36 17.66 18.00 18.36 19.20 20.12 21.30 21.64 23.34 23.98 24.54 25.06 25.88 27.46

27.88 28.18 28.74 29.36 30.28

30.66 31.46 32.02 32.74 33.08 34.08 35.14 35.66 35.74 36.42

36.88 37.50 37.90 37.96 38.46

38.54 39.00 39.36 39.96 40.38 40.64 40.76 41.10 41.20 41.50

2. Phenobarbitone 3. Luminal 4. Phenemal 5. Pheneplethylmalonylurea 8. 8.66 30 1 0 0 7.66 10 0 1 1 1 10 12 12 10 12 12 12 12 12 12 12 12 12 12 12 12 12	Synonyms	Calc	ulated Pa	attern	(Pea	ık h	eight	ts)
S. Phenylethylmalonylurea	3. Luminal		I		hkl		λ - :	20(1.54
CAS registry no. 50-06-6		1			_			9. 11.
Monoclinic, P2/c (14), Z = 4. The structure was determined by Williams [1974].	50-06-6	7.10 6.82	40 51	1 -1	1 1	0 1		12. 12. 14.
Atom positions All atoms are in general positions 4(e) [ibid.]. All atoms are in general positions 4(e) [ibid.]. Polymorphism There may be as many as 12 anhydrous forms of phenobarbital, as well as the monohydrate and perhaps other hydrates [ibid.]. Lattice constants a = 9.539(2) Å b = 11.856(3) c = 10.799(3) β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.535(2), β = 111.56(1)° (published values: a = 9.535(2), β = 111.56(1)° (published values: a = 9.536(2), β = 111.56(1)° (published values: a = 9.536(2), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.856(3), c = 9.535(2), β = 111.56(1)°; sp. gp. P21/a; a/b = 0.9105; c/b = 0.8042 Volume (1135.0 Å Density (calculated) 1.359 g/cm³ Thermal parameters Isotropic for hydrogen atoms [Williams, 1974]. Isotropic for hydrogen atoms, estimated from U ₁ for each atom. Scattering factors (o', Hi'), N'O, O' [International Tables, 1962] Scale factors (integrated intensities) γ = 1.581 x 10 ⁻³ 1/I cornulum (calculated) 0.610 for reflection with hk2 = 202 Additional pattern 1. PDF card 5-0324 [Huang, 1951] References Huang, TY. (1951). Acta Pharm. Int. 2, 43. Lattice constants 4.619 3 0 0 1 2 1 15 4.410 15 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 - 2 1 1 22 4.410 17 -	Monoclinic, $P2_1/c$ (14), $Z = 4$. The structure	5.104	86	0	2	1		16. 17. 17.
There may be as many as 12 anhydrous forms of phenobarbital, as well as the monohydrate and perhaps other hydrates [ibid.]. Lattice constants a = 9.535(2) Å b = 11.856(3) c = 10.795(3) β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° [williams, 1974]) CD cell: a = 10.795(3) Å, b = 11.856(3), c = 9.535(2), β = 111.56(1)°; sp. gp. P2₁/a; a/b = 0.9105; c/b = 0.8042 Volume 1135.0 Å Density (calculated) 1.359 g/cm³ Thermal parameters Isotropic B, for other atoms, estimated from U, j for each atom. Scattering factors CO, H°, N°, N°, 0° [International Tables, 1962] Scale factors (integrated intensities) γ = 1.581 x 10⁻3 I/I corundum (calculated) 0.610 for reflection with kk2 = 202 Additional pattern 1. PDF card 5-0324 [Huang, 1951] References Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.		4.924	14	1	2	0		18. 18.
Lattice constants a = 9.535(2) Å b = 11.856(3) c = 10.795(3) β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° (published values: a = 9.534(2) Å, b = 11.856(3), a	There may be as many as 12 anhydrous forms of phenobarbital, as well as the monohydrate and	4.410 4.168 4.103	15 100 48	-2 -2 1	1 0 2	1 2 1		19. 20. 21. 21. 23.
b = 11.855(3), c = 10.794(3), β = 111.56(1)° [Williams, 1974]) CD cell: a = 10.795(3) Å, b = 11.856(3), c = 9.535(2), β = 111.56(1)°; sp. gp. P2 ₁ /a; a/b = 0.9105; c/b = 0.8042 Volume 0 1135.0 Å Density (calculated) 1.359 g/cm³ Thermal parameters 1	a = 9.535(2) Å b = 11.856(3) c = 10.795(3)	3.708 3.625 3.551 3.440	14 3 10 17	1 2 2	1 2 1	2 0 1		23. 24. 25. 25. 27.
A/b = 0.9105; c/b = 0.8042	b = 11.855(3), c = 10.794(3), β = 111.56(1)° [Williams, 1974]) CD cell: a = 10.795(3) Å, b = 11.856(3),	3.164 3.104 3.040	3 40 2	-1 0 -2	3 3 3	2 2 1		27. 28. 28. 29.
Calculated) 1.359 g/cm ³ Thermal parameters Isotropic for hydrogen atoms [Williams, 1974]. Isotropic B _i for other atoms, estimated from U _{ij} for each atom. Scattering factors C ⁰ , H ⁰ , N ⁰ , 0 ⁰ [International Tables, 1962] Scale factors (integrated intensities) γ = 1.581 x 10 ⁻³ I/I corundum (calculated) 0.610 for reflection with hk\(\partial = \frac{2}{2}\) With hk\(\partial = \frac{2}{2}\) Additional pattern 1. PDF card 5-0324 [Huang, 1951] References Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.	Volume o	2.841 2.793 2.733	2 2 5	0 -3 1	4 2 1	1 1+ 3		30. 31. 32. 32.
Scattering factors Co, Ho, No, Oo [International Tables, 1962] 2.435 4 -3 3 2 36 2.396 6 -3 0 4 37 3 2 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 2 1 37 3 3 3 2 1 37 3 3 3 3 3 3 3 3	(calculated) 1.359 g/cm ³ Thermal parameters	2.629 2.552 2.516	4 3 4	1 0 -3	4 4 2	1 2+ 3		34. 35. 35.
Scattering factors C ⁰ , H ⁰ , N ⁰ , 0 ⁰ [International Tables, 1962] Scale factors (integrated intensities) y = 1.581 x 10 ⁻³ I/I corundum (calculated) 0.610 for reflection with hkl = 202 Additional pattern 1. PDF card 5-0324 [Huang, 1951] References Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.	Isotropic B, for other atoms, estimated from U, for each atom.							36.
Y = 1.581 x 10 ⁻³ 2.339 3 1 4 2 36 I/I corundum_ (calculated) 0.610 for reflection with hkl = 202 2.334 4 -4 1 2 38 38 with hkl = 202 2.308 1 2 3 2+ 39 2.287 7 -1 4 3+ 39 39 Additional pattern 1. PDF card 5-0324 [Huang, 1951] 2.254 2 2 1 3 39 2.232 3 -4 1 3 39 References Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr. 2.218 1 0 4 3+ 40 40 2.111 (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr. 2.174 2 1 1 4+ 41	C ⁰ , H ⁰ , N ⁰ , O ⁰ [International Tables, 1962]	2.396 2.372	6 3 2	-3 3 3	0 2 3	4 1 0		36. 37. 37.
Additional pattern 1. PDF card 5-0324 [Huang, 1951] References Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.	$\gamma = 1.581 \times 10^{-3}$ I/I corundum (calculated) 0.610 for reflection	2.334 2.308	4	-4 2	1 3	2 2+		38. 38.
Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.		2.254	2	2	1	3		39. 39. 40.
	Huang, TY. (1951). Acta Pharm. Int. 2, 43. International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202. Williams, P. P. (1974). Acta Crystallogr.	2.212 2.194 2.189	2 2 2	1 -2 1	0 3 5	4+ 4 1+		40. 40. 41. 41.

Phenobarbital, form III, $C_{12}H_{12}N_2O_3$ - (continued)

2.101 2.084 2.076	2 1 1 1 2	-1 -4 3 -2	1 0 2	5 4	2Θ(°) λ - 1.540598A 43.02 43.38
2.101 2.084 2.076	1 1 1	-4 3	0		λ - 1.540598A 43.02
2.084 2.076	1 1 1	-4 3	0		
2.084 2.076	1 1 1	-4 3	0		
2.076	1 1	3		4	//2 20
	1		2		
		-2		2+	43.56
2.061	2	_	5	2	43.90
2.053		-4	1	4	44.08
2.036	2	-4	3	2	44.46
2.009	1	-1	2	5	45.10
1.980	4	2	5	1+	45.80
1.975	3	0	6	0+	45.90
1.967	3	-4	2	4	46.12
1.907	3	-4	2	4	40.12
1.933	5	3	3	2+	46.98
1.898	1	-3	5	1	47.88
1.878	1	-1	3	5+	48.44
1.873		3	1	3	48.58
1.855	2 2	- 5	1	3	49.06
1.846	4	-4	1	5	49.34
1.841	3	0	6	2	49.46
1.813	1	2	4	3+	50.30
1.804	1	2	6	0	50.54
1.798	2	1	1	5+	50.72
1.773	1	5	0	0+	51.50
	1				
1.754		1	6	2+	52.10
1.732	1	2	6	1+	52.82
1.715	1	- 5	2	4+	53.38
1.685	1	-3	4	5	54.42
1.671	1	-4	5	1+	54.90
1.651	2	- 5	1	5+	55.62
1.639	1	3	0	4	56.06
1.592	1	-2	5	5+	57.86
1.582	1	2	7	0+	58.28

	culated I	Pattern	(I	nte	grated)
d(A)	I		hkl		2Θ(°) 。
					λ - 1.540598A
8.87	28	1	0	0	9.97
7.66	9	0	1	1	11.54
7.10	36	1	1	0	12.45
6.82	47	-1	1	1	12.97
5.93	2	0	2	0	14.93
5.278	38	-1	0	2	16.78
5.129	13	1	1	1	17.27
5.105	76	0	2	1	17.36
5.020	39	0	0	2	17.65
4.928	11	1	2	0	17.98
4.831	5	-1	2	1	18.35
4.822	2	-1	1	2	18.38
4.623	2	0	1	2	19.18
4.434	1	2	0	0	20.01
4.411	14	-2	1	1	20.11

d(A)	I	hkl	2Θ(°) ° λ - 1.540598A
4.169 4.105 3.809 3.708 3.627	100 45 15 15	-2 0 2 1 2 1 1 0 2 -2 2 1 1 1 2	21.29 21.63 23.33 23.98 24.53
3.551	10	2 2 0	25.06
3.443	3	-1 1 3	25.86
3.442	15	2 1 1	25.86
3.246	3	1 3 1	27.46
3.205	5	1 2 2	27.82
3.199	25	-2 1 3 -1 3 2 0 3 2 -3 0 2 -1 2 3	27.87
3.164	1		28.19
3.105	41		28.73
3.092	9		28.85
3.076	1		29.01
3.075	5	2 2 1	29.01
3.039	1	-2 3 1	29.37
2.956	3	3 0 0	30.21
2.950	26	2 3 0	30.27
2.914	4	0 2 3	30.65
2.843 2.794 2.741 2.733 2.706	2 2 1 5	0 4 1 -3 2 1 -3 2 2 1 1 3 -3 1 3	31.44 32.00 32.64 32.74 33.08
2.639	1	-2 0 4	33.94
2.629	4	1 4 1	34.08
2.554	1	0 3 3	35.11
2.552	2	0 4 2	35.13
2.517	4	-3 2 3	35.65
2.510	3	0 0 4	35.75
2.472	4	-3 3 1	36.31
2.464	7	2 4 0	36.43
2.435	4	-3 3 2	36.88
2.396	6	-3 0 4	37.50
2.373	2	3 2 1	37.88
2.367	1	3 3 0	37.98
2.339	5	1 4 2	38.45
2.330	2	-4 1 2	38.61
2.288	5	-1 4 3	39.35
2.287 2.254 2.232 2.219 2.211	3 2 3 1	2 4 1 2 1 3 -4 1 3 0 4 3 1 0 4	39.36 39.96 40.39 40.63 40.77
2.195	2	-2 3 4	41.09
2.189	1	1 5 1	41.21
2.178	1	3 1 2	41.42
2.174	1	1 1 4	41.50
2.101	2	-1 1 5	43.02

Phenobarbital, form III, $C_{12}H_{12}N_2O_3$ - (continued)

d(Å)	Ι	hkl	2Θ(°) 。 λ - 1.540598A
2.085	1	-4 0 4	43.37
2.061	1	-2 5 2	43.89
2.053	2	-4 1 4	44.07
2.036	2	-4 3 2	44.45
2.008	1	-1 2 5	45.11
1.980	3	2 5 1	45.80
1.976	1	0 6 0	45.89
1.971	1	-2 4 4	46.01
1.967	2	-4 2 4	46.12
1.933	4	3 3 2	46.97
1.930	1	1 3 4	47.05
1.898	1	-3 5 1	47.88
1.878	1	-1 3 5	48.43
1.873	2	3 1 3	48.58
1.855	2	-5 1 3	49.06
1.846	4	-4 1 5 0 6 2 2 6 0 1 1 5 2 6 1	49.33
1.839	1		49.54
1.805	1		50.53
1.799	2		50.72
1.732	1		52.82
1.684	1	-3 4 5	54.43
1.671	1	-4 5 1	54.91
1.651	2	-5 1 5	55.61
1.649	1	2 5 3	55.68

Structure Monoclinic, C2/m (12), Z = 2. The structure was refined using data from a natural mineral found in the Kimberley Division of Western Australia [Bagshaw et al., 1977]. Electron microprobe analysis gave the composition listed [ibid.].
Atom positions Bagshaw et al. [1977]
2(a) 2 oxygen 4(i) 4 oxygen in each of 6 different sites 4(i) 3.72 titanium and 0.24 iron in each of 3 different sites 4(i) 2.32 potassium and 1.44 barium
1
Lattice constants o a = 15.454(2) A
b = 3.8370(7) c = 9.124(2) β = 99.25(1)°
a/b = 4.0276 c/b = 2.3779
(published values: $a = 15.453(2) \stackrel{\circ}{A}$, $b = 3.8368(7)$, $c = 9.123(2)$, $\beta = 99.25(1)^{\circ}$ [Bagshaw et al., 1977].
Volume 533.99 A ³
Density 3.978 g/cm ³
Thermal parameters $ \begin{array}{ccccccccccccccccccccccccccccccccccc$
Scattering factors K+, Ba ²⁺ , Fe ⁰ , Ti ⁰ , O ⁰ [Cromer and Mann, 1968]. K, Ba, Fe and Ti factors were corrected for dispersion [Cromer, 1965].
Scale factors (integrated intensities)
$\gamma = 0.1046 \times 10^{-3}$ I/I (calculated) = 1.06 for reflection with hk2 = 310.
References
Bagshaw, A. N., Doran, B. H., White, A. H., and Willis, A. C. (1977). Aust. J. Chem. <u>30</u> , 1195. Cromer, D. T. (1965). Acta Crystallogr. <u>18</u> ,
17. Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. <u>A24</u> , 321.

Cal	lculated	Pattern	(Pe	ak h	eights)
d(A)	I		hkl		2Θ(°) λ - 1.540598A
9.000	7	0	0	1	9.82
7.622	54	2	0	0	11.60
6.339	41	-2	0	1	13.96
5.401	10	2	0	1	16.40
4.498	33	0	0	2	19.72
4.180	1	-2	0	2	21.24
3.811	1	4	0	0	23.32
3.729	23	-4	0	1+	23.84
3.630	7	2	0	2	24.50
3.324	5	4	0	1	26.80
3.171	14	-4	0	2	28.12
3.062	96	3	1	0	29.14
2.988	100	-3	1	1	29.88
2.959	68	-2	0	3	30.18
2.925	30	-1	1	2	30.54
2.815	82	1	1	2+	31.76
2.703	44	4	ō	2	33.12
2.653	26	-3		2+	33.76
	30	-6			
2.556				1	35.08
2.425	2	3	1	2	37.04
2.383	11	-1	1	3+	37.72
2.349	4	6		1	38.28
2.251	5	0	0	4+	40.02
2.239	10	5	1	1	40.24
2.115	4	-6	0	3	42.72
2.092	52	-4	0	4	43.22
2.075	47	6	0	2	43.58
2.047	14	3	1	3	44.22
1.9952	11	- 5	1	3	45.42
1.9602	7	-1	ì	4	46.28
1.9187	59	0	2	0	47.34
1.8939	11	1	1	4+	48.00
1.8604	2	2	2	0	48.92
1.8378	5	- 6	ō	4+	49.56
1.8145	2	4	0	4	50.24
1.8038	14	7	1	1+	50.56
1.7641	7	ó	2	2+	51.78
1.7515	9	- 5	1	4	
					52.18
1.7138	7	- 7	1	3	53.42
1.7067	4	-4	2	1	53.66
1.6961	2	2 2	2	2	54.02
1.6927	1	2	0	5	54.14
1.6649	8	7	1	2	55.12
1.6615	6	4	2	1+	55.24
1.6419	3	-4	2	2	55.96
1.6227	4	- 3	1	5	56.68
1.6164	4	0		3	56.92
1.6097	14	-2		3	57.18
1.5964	5	1	1	5+	57.70
1.5859	. 4	-8	0	4	58.12

Potassium Barium Iron Titanium Oxide, $K_{1.16}Ba_{0.72}Fe_{0.36}Ti_{5.58}O_{13}$ - (continued)

1.5643 16 4 2 1.5609 18 -7 1 1.5547 6 2 2	2 59.00 4 59.14 3 59.40
1.5547 6 2 2	3 50 40
	3 39.40
1.5505 7 9 1	0 59.58
1.5346 20 -6 2	1+ 60.26
1.5254 5 10 0	0 60.66
1.5209 14 -10 0	2 60.86
1.5097 5 7 1	3 61.36
1.5009 10 0 0	6 61.76

	Calculated	Pattern	(I	nte	grated)
d(A)	I	ı	ıkl		2Θ(°)
					λ - 1.540598Α
9.005	6	0	0	1	9.81
7.627	48	2	0	0	11.59
6.345	38	-2	0	1	13.95
5.407	7 9	2	0	1	16.38
4.503	33	0	0	2	19.70
4.183	3 1	-2	0	2	21.22
3.813	3 1	4	0	0	23.31
3.734	20	-4	0	1	23.81
3.72	8	1	1	0	23.89
3.630) 7	2	0	2	24.50
3.325	5 5	4	0	1	26.79
3.172		-4	0	2	28.11
3.063		3	1	0	29.13
3.002	2 9	0	0	3	29.74
2.989		-3	1	1	29.87
2.960) 66	-2	0	3	30.17
2.925		-1	1	2	30.54
2.818		3	1	1	31.73
2.815		1	1	2	31.77
2.70		4	0	2	33.11
2.65	5 18	-3	1	2	33.73
2.652		2	0	3	33.77
2.556		-6	0	1	35.07
2.426		3	1	2	37.03
2.38		- 5	1	1	37.71
2.38	2 8	-1	1	3	37.73
2.350) 4	6	0	1	38.27
2.260		-2	0	4	39.85
2.25		-3	1	3	39.93
2.25		0	0	4	40.02
2.23	9 10	5	1	1	40.24
2.11		-6	0	3	42.72
2.09		-4	0	4	43.22
2.07		6	0	2	43.57
		3	1	3	44.21

d(A)	I	1	hkl		2θ(°) λ - 1.540598Å
1.9950 1.9606 1.9292 1.9185 1.9087	13 7 1 69 4	-5 -1 -8 0 -7	1 1 0 2	3 4 1 0	45.43 46.27 47.07 47.35 47.60
1.9041	1	-3	1	4	47.73
1.8948	3	7	1	0	47.97
1.8936	9	1	1	4	48.01
1.8605	1	2	2	0	48.92
1.8385	4	-6	0	4	49.54
1.8364	2	-2	2	1	49.60
1.8151	1	4	0	4	50.22
1.8081	1	2	2	1	50.43
1.8073	8	8	0	1	50.45
1.8041	10	7	1	1	50.55
1.8023	2	6	0	3	50.60
1.7650	4	0	2	2	51.75
1.7637	4	5	1	3	51.79
1.7518	10	-5	1	4	52.17
1.7141	8	-7	1	3	53.41
1.7064	4	-4	2	1	53.67
1.6962	1	2	2	2	54.02
1.6930	1	2	0	5	54.13
1.6652	10	7	1	2	55.11
1.6617	1	4	2	1	55.23
1.6416	3	-4	2	2	55.97
1.6227	4	-3	1	5	56.68
1.6165	3	0	2	3	56.92
1.6099	17	-2	2	3	57.17
1.5968	5	1	1	5	57.69
1.5956 1.5861 1.5668 1.5652 1.5646	1 4 5 1	-6 -8 -9 6 4	0 0 1 0 2	5 4 1 4 2	57.73 58.11 58.90 58.96 58.99
1.5612	12	-7	1	4	59.13
1.5544	4	2	2	3	59.42
1.5503	5	9	1	0	59.59
1.5371	7	-9	1	2	60.15
1.5360	12	4	0	5	60.20
1.5344	13	-6	2	1	60.27
1.5337	2	-5	1	5	60.30
1.5253	3	10	0	0	60.66
1.5209	13	-10	0	2	60.86
1.5197	2	-2	0	6	60.91
1.5099	5 12	7 0	1 0	3 6	61.35 61.76

Synonyms

- 1. Novocaine hydrochloride
- p-Aminobenzoyldiethylaminoethanol hydrochloride
- 2-Diethylaminoethyl p-aminobenzoate hydrochloride

CAS registry no. 51-05-8

Structure

Orthorhombic, Pcab (61), Z = 8. The structure was studied by Beall, Herdklotz and Sass [1970]. The parameters used here are from the refinement by Dexter [1972].

Atom positions

All atoms were in the general positions 8(c) [Dexter, 1972].

Lattice constants

a = 25.019(1) Ab = 8.3060(5)

c = 14.193(1)

(published values: $a = 25.017(1) \stackrel{\circ}{A}$, b = 8.3050(5), c = 14.192(1) [Dexter, 1972])

CD cell: $a = 14.193(1) \stackrel{\circ}{A}$, b = 25.019(1), c = 8.3060(5); sp. gp. Pcab; a/b = 0.5673; c/b = 0.3320

Volume o 2949.4 A³

Density

(calculated) 1.229 g/cm³

Thermal parameters

Isotropic: hydrogen atoms, overall B = 4.0
[Dexter, 1972].
Isotropic B. for other atoms, estimated from
U. for each atom.

Scattering factors

 C^0 , H^0 , N^0 , O^0 , Cl^- [International Tables, 1962]

Scale factors (integrated intensities)

 $\gamma = 0.5173 \times 10^{-3}$

 $I/I_{corundum}$ (calculated) = 0.601, for reflection with hk2 = 113.

Additional patterns

- 1. PDF card 27-1975 [Wang, P. Polytechnic Inst. of New York, 1975]
- 2. Folen [1975]

References

Beall, E., Herdklotz, J., and Sass, R. L. (1970). Biochem. Biophys. Res. Commun. 39, 329.

Dexter, D. D. (1972). Acta Crystallogr. <u>B28</u>, 77. Folen, V. A. (1975). J. Forensic Sci. <u>20</u>, 348. <u>International Tables for X-ray Crystallography</u>, <u>III</u> (1962). (The Kynoch Press, Birmingham, <u>Eng.</u>) p. 202.

0	urated	Pattern	(Pe	ak r	eignus)
d(A)	Ι		hkl		2Θ(°) λ - 1.540598 <i>i</i>
12.51	7	2		0	7.06
7.09	6	0		2	12.48
6.89	35	1	1	1	12.84
6.22 5.434	37 79	2	1 1	1+ 1	14.22 16.30
5.401	66	0	1	2	16.40
4.951	4	2		2	17.90
4.692	7	4		2	18.90
4.423 4.153	16 59	2		3 0	20.06 21.38
4.100	33	5	1	1	21.66
4.055	100	1		3	21.90
3.9039	28	2		3	22.76
3.7954	2	2		1	23.42
3.7171	18	3	2	0	23.92
3.6688	16	5		2	24.24
3.6015 3.5478	9 24	6		1 4	24.70 25.08
3.4347	6	4		3	25.92
3.4140	4	2		4	26.08
3.3608	3	4	2	1	26.50
3.2925	4	6		2+	27.06
3.2618	15	0		4	27.32
3.2362 3.1975	8 17	1 7	1 1	4	27.54 27.88
		/	1		
3.1752	31	5		3	28.08
3.1272 3.0953	15 22	6 1		3+ 3	28.52 28.82
3.0275	3	2		3	29.48
2.9781	2	7		2	29.98
2.9229	9	3	2	3+	30.56
2.8662	5	8		1	31.18
2.7929	2	4		3	32.02
2.7677 2.7170	1 3	2		5 2	32.32 32.94
2.6979					
2.6483	12 10	0 5		4+ 3	33.18 33.82
2.6079	3	8		3	34.36
2.5788	15	0		2+	34.76
2.5253	6	2		2	35.52
2.4927	6	4	3	1+	36.00
2.4702	3	9	1	2	36.34
2.4650	3	10		1	36.42
2.3781 2.3612	2 4	1 5		3 5+	37.80 38.08

Procaine Hydrochloride, $C_{13}H_{21}C1N_2O_2$ - (continued)

d(A)	I	hkl 2Θ(°) (λ - 1.540598	À
2.3470	6	2 3 3+ 38.32	
2.3019	2	9 1 3+ 39.10	
2.2929	3	5 3 2 39.26	
2.2762	5	6 3 1+ 39.56	
2.2652	5	1 1 6+ 39.76	
2.2587	5	6 1 5 39.88	1
2.2109	1	10 0 3 40.78	
2.1934	2	6 3 2+ 41.12	
2.1822	3	0 3 4 41.34	
2.1436	2	7 1 5+ 42.12	
2.0907	1	7 3 2 43.24	
2.0851	2	12 0 0 43.36	
2.0769	2	0 4 0 43.54	
2.0439	4	10 0 4+ 44.28	
2.0283	1	2 2 6+ 44.64	
1.9952 1.9903 1.9594 1.9318 1.9179	3 3 2 1	11 2 0+ 45.42 11 1 3+ 45.54 7 2 5 46.30 9 1 5+ 47.00 5 4 0+ 47.36	
1.8991	2	8 3 3+ 47.86	
1.8582	1	13 1 1+ 48.98	
1.8540	1	3 4 3 49.10	
1.8385	2	10 3 1+ 49.54	
1.8344	2	5 1 7+ 49.66	
1.8166	1	1 2 7 50.18	
1.8125	2	13 1 2 50.30	
1.7978	3	0 3 6+ 50.74	
1.7899	4	6 3 5+ 50.98	
1.7814	3	7 4 1+ 51.24	
1.7776	2	5 4 3+ 51.36	
1.7566	1	2 0 8+ 52.02	
1.7429	2	13 1 3+ 52.46	
1.7300	2	1 1 8+ 52.88	
1.7120	2	5 2 7+ 53.48	
1.7073 1.6392 1.6280 1.6222 1.6180	2 2 1 2	4 0 8 53.64 5 1 8+ 56.06 1 2 8 56.48 2 3 7+ 56.70 3 5 1+ 56.86	
1.6040	1	2 5 2+ 57.40	
1.5667	2	5 5 1+ 58.90	
1.5600	1	0 4 6+ 59.18	
1.5547	1	10 3 5+ 59.40	

	Calculated	Pattern	(II	itegi	cated)
d(Å)	Ι	ŀ	ıkl)	20(°) ° \ - 1.540598A
12.51 7.10 6.89 6.25 6.22	7 5 33 22 23	2 0 1 4 2	0 0 1 0	0 2 1 0	7.06 12.46 12.84 14.15 14.23
6.17 5.436 5.395 4.954	5 48 4 4	2 3 0 2 4	0 1 1 1 1	2 1 2 2 1	14.34 16.29 16.42 17.89 18.81
4.692 4.425 4.153 4.103 4.097	5 15 3 58 3 21	4 2 0 5 1	0 0 2 1 2	2 3 0 1 0	18.90 20.05 21.38 21.64 21.67
4.085 4.057 4.001 3.941 3.936	7 100 1 4 15 1	4 1 6 2 1	1 1 0 2 2	2 3 1 0 1	21.74 21.89 22.20 22.54 22.57
3.905 3.797 3.717 3.687 3.668	77 1 76 17 73 9	2 2 3 3 5	1 2 2 1 1	3 1 0 3 2	22.75 23.41 23.92 24.12 24.24
3.604 3.584 3.548 3.435 3.413	43 2 82 25 53 5	6 0 0 4 2	1 2 0 1	1 2 4 3 4	24.68 24.82 25.08 25.91 26.08
3.363 3.299 3.293 3.263 3.235	93 2 31 1 30 15	4 6 3 0 1	2 1 2 1 1	1 2 2 4 4	26.50 27.00 27.06 27.31 27.55
3.198 3.176 3.157 3.128 3.12	64 31 73 2 82 8	7 5 2 6 8	1 1 1 0 0	1 3 4 3 0	27.87 28.07 28.24 28.51 28.52
3.11 3.09 3.086 3.028 2.979	71 22 62 2 82 2	5 1 4 2 7	2 2 0 2 1	1 3 4 3 2	28.61 28.80 28.91 29.47 29.96
2.94; 2.92; 2.91; 2.866 2.79;	31 9 39 3 65 5	6 3 5 8 4	2 2 2 1 2	0 3 2 1 3	30.35 30.56 30.66 31.18 32.02

Procaine Hydrochloride, $C_{13}H_{21}ClN_2O_2$ - (continued)

d(Å)	I	, hkl	2Θ(°) λ - 1.540598Å
2.7682	1	2 0 5	32.31
2.7181	2	6 2 2	32.93
2.7016	1	1 3 1	33.13
2.6977	9	0 2 4	33.18
2.6973	3	7 1 3	33.19
2.6822	4	1 2 4	33.38
2.6610	4	7 2 1	33.65
2.6482	10	5 2 3	33.82
2.6371	1	2 2 4	33.97
2.6089	2	8 0 3	34.35
2.5849	5	4 0 5	34.68
2.5793	13	0 3 2	34.75
2.5668	4	3 2 4	34.93
2.5567	3	3 1 5	35.07
2.5309	1	7 2 2	35.44
2.5262	5	2 3 2	35.51
2.5019	4	10 0 0	35.86
2.4987	1	6 2 3	35.91
2.4924	4	4 3 1	36.01
2.4712	2	9 1 2	36.33
2.4639	1	10 0 1	36.44
2.3880	1	5 3 1	37.64
2.3787	2	1 3 3	37.79
2.3666	2	5 1 5	37.99
2.3622	2	10 1 1	38.06
2.3471	4	2 3 3	38.32
2.3465	2	6 0 5	38.33
2.3028	1	9 1 3	39.08
2.2926	2	5 3 2	39.27
2.2801	1	9 2 1	39.49
2.2767	4	6 3 1	39.55
2.2750	1	0 1 6	39.58
2.2657	3	1 1 6	39.75
2.2650	1	6 2 4	39.76
2.2581	3	6 1 5	39.89
2.2117 2.1936 2.1828 2.1473 2.1431	1 1 3 1	10 0 3 6 3 2 0 3 4 7 1 5 10 2 0	40.77 41.12 41.33 42.04 42.13
2.0916	1	7 3 2	43.22
2.0849	1	12 0 0	43.36
2.0765	2	0 4 0	43.55
2.0486	1	1 2 6	44.17
2.0447	3	10 0 4	44.26
2.0430	1	6 2 5	44.30
1.9971	1	6 1 6	45.37
1.9949	2	11 2 0	45.43
1.9902	2	11 1 3	45.54
1.9598	2	7 2 5	46.29

d(Å)	I		hkl		2Θ(°) ° λ - 1.540598Å
1.9317	1	9	1	5	47.00
1.9179	1	5	4	0	47.36
1.8987	2	8	3	3	47.87
1.8587	1	13		1	48.97
1.8538	1	3	4	3	49.10
1.8430	1	6	4	1	49.41
1.8406	1	10	3	1	49.48
1.8381	1	11	2	3	49.55
1.8172	1	1	2	7	50.16
1.8127	2	13	1	2	50.30
1.7985	2	0	3	6	50.72
1.7901	3	6	3	5	50.98
1.7876	1	1	4	4	51.05
1.7813	1	7	4	1	51.25
1.7774	1	5	4	3	51.36
1.7462	1	13	2	0	52.35
1.7430	2	13	1	3	52.46
1.7308	1	1.	1	8	52.85
1.7121	2	5	2	7	53.48
1.7068	1	4	0	8	53.66
1.6392	1	5	1	8	56.06
1.6323	1	1	3	7	56.32
1.6280	1	1	2	8	56.48
1.6220	1	2	3	7	56.71
1.6041	1	2	5	2	57.40
1.5670	1	5	5	1	58.89
1.5667	1	13	2	4	58.90

Synonyms

1. 3-(2-(Dimethylamino)ethyl)-indol-4-ol

2. 4-Hydroxy-N, N-dimethyltryptamine

CAS registry no. 520-53-6

Structure

Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Petcher and Weber [1974].

Atom positions

All the atoms were in general positions 4(e). For H(7), the value 0.273 was used for "z" as given in the Supplementary Publ. #SUP20980, referred to by Petcher and Weber [1974]. Bond length calculations indicated that the value of 0.014 for "z" for H(12) should be used.

Lattice constants

a = 10.60(3) Å b = 8.53(2) c = 12.51(3) β = 91.25(30)° [Petcher and Weber, 1974]

[Petcher and Weber, 1974]

CD cell: a = 12.51(3) Å, b = 8.53(2), $c = 10.60(3), \beta = 91.25(30)^{\circ}; \text{ sp. gp. } P2_{1}/a;$ a/b = 1.4665, c/b = 1.2426

Volume 0 1131. A³

Density (calculated) 1.200 g/cm³

(measured) 1.19 [Petcher and Weber, 1974]

Thermal parameters

Isotropic B_i estimated from β_{ij} for individual atoms.

Scattering factors

Zero ionization [International Tables, 1962]

Scale factors (integrated intensities) $\gamma = 3.259 \times 10^{-3}$

 $I/I_{corundum}$ (calculated) = 1.06 for reflection with hk ℓ = 112.

Additional pattern

1. PDF card 13-981 [Physical Data of Indole and Dihydroindole Alkaloids, edited by Neuss, Eli Lilly and Co., 1962]

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Petcher, T. J. and Weber, H. P. (1974).
J. Chem. Soc. Perkin Trans. 2, 946.

	culated	Pattern	(Pe	ак п	eigi	nts)
d(A)	I		hkl		λ -	20(°) 1.540598A
10.59	51	1	0	0		8.34
7.04	10	0	1	1		12.56
6.64	6	1	1	0		13.32
6.25	1	0	0	2		14.16
5.89	5	-1	1	1		15.02
5.83	9	1	1	1		15.18
5.43	2	-1	0	2		16.30
5.30	22	2	0	0		16.72 17.58
5.04 4.58	12 33	0 -1	1 1	2		17.36
4.52 4.26	100	1 0	1 2	2. 0		19.62 20.82
4.20	22 21	2	1	1		21.10
4.08	4	-2	0	2		21.74
4.00	3	2	ő	2		22.22
3.96	6	1	2	0		22.46
3.76	47	1	2	1		23.64
3.62	2	2	1	2		24.56
3.51	2	1	1	3		25.36
3.33	9	1	2	2		26.74
3.26	1	3	1	0		27.32
3.20	5	2		1		27.86
3.09	1	-2		3 2		28.90
3.05	2	3				29.30
2.934	4	0	1	4		30.44
2.917	6	2	2	2		30.62
2.857	5	1		3		31.28
2.773	5 2	0		1		32.26
2.746	2	1		0		32.58
2.648	1	3	2	1		33.82
2.615	2	-2	2	3		34.26
2.509	6	1		2+		35.76
2.479	1	3	2	2		36.20
2.461	2	-2	. 3	1+		36.48
2.443	2	1	2	4		36.76
2.367	1	-3	0	4		37.98
2.317	1	2	. 3	2+		38.84
2.281	1	-3		4		39.48
2.261	2	2		4		39.84
2.207	1	4	2	1		40.86
2.138	1	2		3		42.24
2.120	2	5	0	0		42.62
2.079	1	3	3	2		43.50
2.043	1	-4		4		44.30
2.018	1	0	4	2		44.88
1.995	2	-4		3+		45.42
1.955	1	-2	. 0	6		46.42
1.945	1	3		3		46.66
1.796	1	3	3	4+		50.80
1.669	1	-3	3	5+		54.96
1.665	1	2	4	4		55.10

Calculated Pattern (Peak heights)

Psilocin, $C_{12}H_{16}N_20$ - (continued)

	Calculated	Patter	n (Int	egrated)
d(A)	I		hkl		2Θ(°) ° λ - 1.540598A
10.60	47	1	0	0	8.34
7.05	10	0	1	1	12.55
6.64	5	1	1	0	13.31
6.25	1	0	0	2	14.15
5.90	4	-1	1	1	15.00
5.84	8	1	1	1	15.17
5.44	1	-1	0	2	16.29
5.34	1	1	0	2	16.60
5.30	21	2	0	0	16.72
5.04	12	0	1	2	17.57
4.59	28	-1	1	2	19.34
4.52	100	1	1	2	19.61
4.50	1	2	1	0	19.71
4.26	18	0	2	0	20.81
4.26	3	-2	1	1	20.83
4.21	20	2	1	1	21.08
4.09	3	-2	0	2	21.73
4.00	3	2	0	2	22.21
3.96	6	1	2	0	22.45
3.76	51	1	2	1	23.62
3.75	1	0	1	3	23.74
3.62	2	2	1	2	24.56
3.51	2	1	1	3	25.35
3.36	2	-1	2	2	26.54
3.33	2	1	2	2	26.74
3.26 3.20 3.09 3.05 3.03	1 5 1 2	3 2 -2 3 2	1 2 1 0 1	0 1 3 2 3	27.30 27.86 28.90 29.28 29.45
2.936	4	0	1	4	30.42
2.918	6	2	2	2	30.62
2.858	6	1	2	3	31.27
2.773	5	0	3	1	32.26
2.746	2	1	3	0	32.58
2.649	1	3	2	1	33.81
2.616	2	-2	2	3	34.25
2.510	1	-3	2	2	35.74
2.509	6	1	3	2	35.76
2.479	1	3	2	2	36.20
2.462 2.444 2.367 2.317 2.281	2 2 1 1	-2 1 -3 2 -3	3 2 0 3 1	1 4 4 2 4	36.47 36.75 37.98 38.83 39.48
2.262	3	2	2	4	39.83
2.208	1	4	2	1	40.84
2.138	1	2	3	3	42.24
2.119	2	5	0	0	42.62
2.079	1	3	3	2	43.50

d(A)	I	ŀ	ıkl		2Θ(°) ° λ - 1.540598A
2.043	1	-4	0	4	44.29
1.996	1	-4	2	3	45.40
1.994	1	5	0	2	45.45
1.954	1	-2	0	6	46.42
1.945	1	3	3	3	46.66
1.796	1	3	3	4	50.80
1.782	1	2	4	3	51.23
1.666	1	2	4	4	55.09

Synonyms	Cal	culated Pa	ttern (Peak	heights)
 Indocybin 3-[2-(Dimethylamino)ethyl]indol-4-ol dihydrogen phosphate methanolate 	d(Å)	I	h	kl	2θ(° λ - 1.54
CAS registry no.	14.52	1	0	2 0	6.
520-52-5	12.07	2	1	0 0	7.:
	11.13	2	1	1 0	7.5
Structure	9.28	100	1	2 0	9
Monoclinic, $P2_1/c$ (14), $Z = 8$. The structure was determined by Weber and Petcher [1974].	8.11	24	0	1 1	10.
	7.56	4	1	3 0	11.
Atom positions	7.27	41	0	4 0+	12.
All atoms were in general positions 4(e).	7.11	74	-1	2 1	12.
	6.23	5	-1	3 1+	14.
Lattice constants	5.98	38	1	1 1	14.
0 - 12 6/(1) 4					
a = 12.64(1) A b = 29.11(2)	5.63	14	1	2 1	15.
c = 8.848(6)	5.51	50	0	4 1	16.
$\beta = 107.37(2)^{\circ}$	5.43	14	-1	4 1	16.
ρ - 107.37(2)	5.24	16		5 0	16.
a/b = 0.4342	5.17	15	1	3 1	17.
c/b = 0.3040					
C/D = 0.3040	4.97	8		3 1	17.
(published values: a = 12.64(1) Å,	4.79	3		5 1	18.
	4.74	2	-1	5 1	18.
$b = 29.11(2), c = 8.847(6), \beta = 107.37(2)^{\circ}$	4.68	3		4 1	18.
[Weber and Petcher, 1974])	4.64	2	2	4 0	19.
Volume o 3107.A ³	4.50	49	1	6 0	19.
3107.A	4.367	30	- 1	1 2	20.
Density	4.283	7	2	1 1	20.
(calculated) 1.352 g/cm ³	4.219	35	0	0 2+	
(measured) 1.34 [Weber and Petcher, 1974]	4.172	42	-1	6 1+	21.:
Thermal parameters	4.096	17	-3		21.
Isotropic, for hydrogens [Weber and Petcher,	4.041	46	-2		
1974]. For all other atoms, B, were estimated	3.983	18		2 1+	
	3.955	15		3 1	22.
for $\beta_{i,j}$ for individual atoms.	3.928	19	1	7 0+	22.
Scattering factors	3.870	16	0	3 2	22.
Zero ionization [International Tables, 1962]	3.779	32		6 0+	
	3.708	18	-1	7 1+	
Scale factors (integrated intensities)	3.657	30		0 2	24.
$\gamma = 0.5540 \times 10^{-3}$ I/I (calculated) = 0.455 for reflection	3.599	11	-3	4 1	24.
with $hk\ell = 120$.	3.556	50	-2	4 2	25.
	3.450	11	-3	1 2	25.
Additional patterns	3.424	10	2		26.
1. PDF card 13-982 [Physical Data of Indole	3.376	5	-2	7 1+	26.
and Dihydroindole Alkaloids edited by Neuss, Eli Lilly and Co., 1962]	3.339	6	0	8 1+	26.
2. Folen [1975]	3.309	4	3	5 0	26.
	3.266	37		4 2+	
References	3.184	2		6 2	28.
Folen, V. A. (1975). J. Forensic Sci. 20, 348.	3.149	3	-3		28.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham,	3.125	4	1	8 1+	
Eng.) p. 202.	3.097	12	1	5 2	28.
Weber, H. P. and Petcher, T. J. (1974). J.	3.019	9	0	9 1+	29.
Chem. Soc. Perkin Trans. 2, p. 942.	3.000	8		1 0+	
<u>-, -</u>	2.953	8		2 0	30.
	2.921	2	1	6 2+	30.5

d	l(Å)	I		hkl	λ -	2θ(°) 。 1.540598A
]]	14.52 12.07 11.13 9.28 8.11	1 2 2 100 24	0 1 1 1 0	2 0 0 0 1 0 2 0 1 1		6.08 7.32 7.94 9.52 10.90
	7.56 7.27 7.11 6.23 5.98	4 41 74 5 38	1 0 -1 -1 1	3 0 4 0+ 2 1 3 1+ 1 1		11.70 12.16 12.44 14.20 14.80
	5.63 5.51 5.43 5.24 5.17	14 50 14 16 15	1 0 -1 1	2 1 4 1 4 1 5 0 3 1		15.72 16.08 16.32 16.90 17.14
	4.97 4.79 4.74 4.68 4.64	8 3 2 3 2	-2 0 -1 1 2	3 1 5 1 5 1 4 1 4 0		17.82 18.50 18.72 18.96 19.10
	4.50 4.367 4.283 4.219 4.172	49 30 7 35 42	1 -1 2 0 -1	6 0 1 2 1 1 0 2+ 6 1+		19.72 20.32 20.72 21.04 21.28
	4.096 4.041 3.983 3.955 3.928	17 46 18 15	-3 -2 -3 2 1	1 1 1 2+ 2 1+ 3 1 7 0+		21.68 21.98 22.30 22.46 22.62
	3.870 3.779 3.708 3.657 3.599	16 32 18 30 11	0 2 -1 1 -3	3 2 6 0+ 7 1+ 0 2 4 1		22.96 23.52 23.98 24.32 24.72
	3.556 3.450 3.424 3.376 3.339	50 11 10 5 6	-2 -3 2 -2 0	4 2 1 2 7 0+ 7 1+ 8 1+		25.02 25.80 26.00 26.38 26.68
	3.309 3.266 3.184 3.149 3.125	4 37 2 3 4	3 1 0 -3 1	5 0 4 2+ 6 2 6 1 8 1+		26.92 27.28 28.00 28.32 28.54
	3.097 3.019 3.000 2.953 2.921	12 9 8 8 2	1 0 4 4 1	5 2 9 1+ 1 0+ 2 0 6 2+		28.80 29.56 29.76 30.24 30.58

d(A)	I	hkl 2Θ(°) o
		λ - 1.540598Α
2.895	6	-4 0 2 30.86
2.882	6	-4 1 2+ 31.00
2.852	4	1 9 1+ 31.34
2.819	4	2 4 2+ 31.72
2.776	3	- 4 3 2+ 32.22
2.,,,	J	. 5 _ 5
2.741	5	- 1 10 1 32.64
2.698	3	- 2 4 3+ 33.18
2.667	2	-3 7 2 33.58
2.618	3	- 3 3 3 34.22
2.611	3	-1 9 2 34.32
2.592	4	2 9 1+ 34.58
2.564	4	4 2 1+ 34.96
2.548		
2.535	3	
	3 4	
2.513	4	-4 7 1+ 35.70
2.490	2	1 3 3+ 36.04
2.462	2	-3 5 3 36.46
2.445	3	-4 1 3+ 36.72
2.434	5	0 6 3 36.90
2.413	3	5 0 0+ 37.24
	•	5 0 0 0 0 7 /0
2.398	2	-5 2 2+ 37.48
2.378	3	4 5 1+ 37.80
2.372	3	-2 10 2+ 37.90
2.341	2	5 3 0+ 38.42
2.327	1	- 4 4 3 38.66
2.319	2	- 5 5 1 38.80
2.290	4	5 4 0+ 39.32
2.270	2	-2 8 3+ 39.68
2.202	2	1 13 0+ 40.96
2.193	4	2 4 3+ 41.12
2.189	4	1 7 3+ 41.20
2.173	2	-5 6 2+ 41.52
2.160	2	-5 7 1+ 41.78
2.140	3	2 5 3+ 42.20
2.126	1	-1 12 2+ 42.48
2.118	1	4 8 1+ 42.66
2.103	i	1 13 1+ 42.98
2.103	•	110 1. 42170

Calculated Pattern (Integrated)						
d(Å)	I		hkl		2Θ(°) ° λ - 1.540598A	
14.55 12.06 11.14 9.29 8.11	1 2 2 100 24	0 1 1 1 0		0 0 0 0 1	6.07 7.32 7.93 9.51 10.90	

d(Å)	I	•	hkl		2Θ(°) ο λ - 1.540598A
7.56	3	1	3	0	11.69
7.30	10	0	2	1	12.11
7.28	31	0	4	0	12.15
7.11	74	-1	2	1	12.43
6.24	3	-1	3	1	14.17
6.23 6.03 5.98 5.68 5.64	2 1 39 5 12	1 2 1 -2 1	4 0 1 1 2	0 0 1 1	14.20 14.67 14.79 15.58 15.71
5.51	52	0	4	1	16.06
5.43	11	-1	4	1	16.31
5.24	16	1	5	0	16.90
5.17	15	1	3	1	17.13
5.12	1	2	3	0	17.30
4.97	8	-2	3	1	17.82
4.79	3	0	5	1	18.50
4.74	1	-1	5	1	18.71
4.68	2	1	4	1	18.94
4.64	1	2	4	0	19.10
4.53	12	-2	4	1	19.57
4.50	51	1	6	0	19.71
4.368	32	-1	1	2	20.32
4.287	5	2	1	1	20.70
4.227	11	-1	2	2	21.00
4.222	23	0	0	2	21.02
4.189	16	2	5	0	21.19
4.179	14	0	1	2	21.25
4.170	23	-1	6	1	21.29
4.154	3	2	2	1	21.37
4.107	3	-2	5	1	21.62
4.101	10	-3	1	1	21.65
4.078	8	-2	0	2	21.78
4.055	26	0	2	2	21.90
4.038	31	-2	1	2	21.99
4.021 4.021 3.984 3.983 3.957	16 4 8 5 10	3 -1 -3 3 2	0 3 2 1 3	0 2 1 0	22.09 22.09 22.30 22.30 22.45
3.932	11	1	7	0	22.60
3.927	7	-2	2	2	22.63
3.872	16	0	3	2	22.95
3.810	4	-3	3	1	23.33
3.800	9	1	6	1	23.39
3.780	24	2	6	0	23.51
3.776	9	-1	4	2	23.54
3.731	5	0	7	1	23.83
3.724	2	2	4	1	23.88
3.715	8	3	3	0	23.94
3.705	10	-1	7	1	24.00
3.659	33	1	0	2	24.31
3.631	2	1	1	2	24.50
3.600	8	-3	4	1	24.71
3.557	57	-2	4	2	25.01

Psilocybin Methanolate, $C_{13}H_{21}N_2O_4P$ - (continued)

d(A)	I	ì	hkl		2Θ(°) λ = 1.560598Δ
					λ - 1.540598Α
3.520	1	3	4	0	25.28
3.519	2	-1	5	2	25.29
3.476	1	-3 -3	0	2	25.61
3.451	11	- 3	1	2	25.79
3.438	2	1	7	1	25.89
3.424	3	1	3	2	26.00
3.424	5	2	7	0	26.00
3.418	1	0	5 2	2	26.05 26.34
3.381 3.378	1 2	-3 -2	7	1	26.34 26.36
3.375	2	- 3	5	1	26.39
3.342	3	0	8	1	26.65 26.67
3.340 3.323	3 2	-2 -1	5 8	2	26.67 26.81
3.323	2	3	5	0	26.93
3.272	1	-3 1	3 4	2	27.23 27.26
3.269 3.266	32 10	-1	6	2	27.26
3.256	10 7	3	1	1	27.28
3.231	2	2	6	1	27.41
3.185	1	0	6	2	27.99
3.150	2	-3	6	1	28.31
3.127	3	1	8	1	28.52
3.098	13	1	5	2	28.79
3.083	3	-4	2	1	28.94
3.081	5	-2	8	1	28.95
3.028	4	-1	7	2	29.48
3.020	7	0	9	1	29.55
3.000	6	4	1	0	29.76
3.000	2	-4	3	1	29.76
2.963	1	0	7	2	30.14
2.953	9	4	2	0	30.24
2.897	5	-4	0	2	30.84
2.883	3	-4	1	2	31.00
2.880	2	4	3	0	31.03
2.859	2	1	9	1	31.26
2.852	2	3	5 2	1	31.34
2.848	1	-2		3	31.38
2.824	2	-2	9	1	31.66
2.818	2	2	4	2	31.72
2.783	1	-2	3	3	32.14
2.776	1	-4	3	2	32.22
2.742	5	-1	10	1	32.64
2.728	1	-1 -2	4	3	32.80
2.698	2	-2	4	3	33.18
2.667	3	-3 1	7	2	33.58
2.628	1	1	10	1	34.09 34.23
2.618	2 2	-3 -1	3	3 2	34.23 34.34
2.610 2.599	1	-1 -2	9 5	3	34.34 34.48
2.399	1	-2	J	3	54.40

d(A)	I	hkl	2Θ(°) λ - 1.540598Å
2.592 2.566 2.564 2.549 2.547	3 2 3 1	2 9 1 1 1 3 4 2 1 -3 9 1 -3 4 3	34.57 34.94 34.97 35.17 35.21
2.537	1	1 2 3	35.35
2.534	1	0 5 3	35.39
2.516	1	-1 6 3	35.66
2.513	1	-3 8 2	35.69
2.513	2	-4 7 1	35.70
2.490	2	1 3 3	36.04
2.463	1	-3 5 3	36.45
2.447	2	-4 1 3	36.70
2.446	1	-5 3 1	36.71
2.435	5	0 6 3	36.89
2.426 2.423 2.413 2.411 2.388	1 1 1 1	0 12 0 1 9 2 5 0 0 3 4 2 -5 4 1	37.03 37.07 37.24 37.26 37.64
2.382 2.377 2.369 2.341 2.327	1 2 1 2	-3 10 1 4 5 1 -2 10 2 5 3 0 -4 4 3	37.74 37.81 37.95 38.41 38.67
2.319	1	-5 5 1	38.81
2.295		4 6 1	39.23
2.290		5 4 0	39.31
2.278		1 10 2	39.53
2.270		-2 8 3	39.67
2.266	1	-4 8 2	39.74
2.202	1	1 13 0	40.96
2.194	2	2 4 3	41.11
2.194	2	-1 0 4	41.11
2.190	1	1 7 3	41.19
2.184	1	-2 2 4	41.31
2.173	1	-5 6 2	41.52
2.160	1	-5 7 1	41.78
2.140	2	2 5 3	42.20
2.126	1	-1 12 2	42.48
2.103	1	1 13 1	42.98

Synonyms 1. Sodium 5,5-diethylbarbiturate 2. Soluble barbital 3. Barbitone sodium 4. Sodium malonylurea
CAS registry no. 144-02-5
Structure Orthorhombic, $P2_12_12_1$ (19), $Z=4$. The structure was determined by Berking and Craven [1971]. It is isostructural with potassium barbital [Berthou et al., 1962].
Atom positions All atoms were in general positions 4(a) [ibid.].
Lattice constants a = 6.724(1) Å b = 11.951(2) c = 12.130(2)
(published values: a = 6.724(1) Å, b = 11.950(2), c = 12.129(2) [Berking and Craven, 1971])
CD cell: a = 11.951(2) Å, b = 12.130(2), c = 6.724(1); sp. gp. P2 ₁ 2 ₁ 2 ₁ ; a/b = 0.9852, c/b = 0.5543
Volume 974.75 A ³
Density (calculated) 1.405 g/cm ³ (measured) 1.408 g/cm ³ [Berking and Craven, 1971]
Thermal parameters Isotropic for hydrogen atoms, anisotropic for non-hydrogen atoms [Berking and Craven, 1971]
Scattering factors C ⁰ , H ⁰ , Na ⁰ , N ⁰ , O ⁰ [International Tables, 1962]
Scale factors (integrated intensities)
Additional pattern 1. PDF card 9-512 [Parkes, E. B., South-Western Forensic Science Lab., Westbury on Trym, Bristol 9, Eng.]
References Berking, B. and Craven, B. M. (1971). Acta Crystallogr. B27, 1107. Berthou, J., Cavelier, C., Marek, D., Rérat, B., and Rérat, C. (1962). C. R. Acad. Sci. 255, 1632.
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	culated	Pattern	(Pea	ak heig	hts)
d(Å)	Ι		hkl	λ -	2Θ(°) 1.540598A
8.50 6.06 5.97 5.85 5.36	100 26 17 65 53	0 0 0 1	1 0 2 1 2	1 2 0 0	10.40 14.60 14.82 15.12 16.54
5.28 4.503 4.255 4.211 3.783	8 6 51 30 9	1 1 0 1	1 0 2 1 3	1 2 2 2+ 1	16.78 19.70 20.86 21.08 23.50
3.596	4	1	2	2	24.74
3.464	4	1	0	3	25.70
3.427	2	1	3	0	25.98
3.329	30	0	3	2+	26.76
3.236	4	2	1	0+	27.54
3.127	27	2	1	1	28.52
3.032	1	0	0	4	29.44
2.986	9	0	4	0+	29.90
2.930	3	2	2	0	30.48
2.901	3	0	4	1	30.80
2.838	16	0	3	3	31.50
2.764	1	1	0	4	32.36
2.693	3	1	1	4	33.24
2.664	6	1	4	1	33.62
2.638	4	2	2	2	33.96
2.614 2.509 2.490 2.403 2.3720	8 5 2 7 3	1 1 0 2	3 2 4 4 2	3 4 2 3 3+	34.28 35.76 36.04 37.40 37.90
2.3446 2.2707 2.2663 2.2522 2.2415	2 5 4 2 4	0 1 1 1	5 3 4 5 1	1 4 3 0+ 5	38.36 39.66 39.74 40.00 40.20
2.2234	1	0	5	2	40.54
2.2140	3	1	5	1+	40.72
2.2026	7	3	1	0+	40.94
2.1672	4	3	1	1+	41.64
2.1074	2	2	2	4+	42.88
2.0679	5	3	2	1	43.74
2.0581	3	0	5	3	43.96
2.0291	5	1	4	4	44.62
1.9804	3	1	3	5	45.78
1.9602	1	2	3	4+	46.28
1.9538	2	3	3	0	46.44
1.9349	2	3	1	3+	46.92
1.8924	2	0	6	2	48.04
1.8865	3	1	6	1	48.20
1.8777	2	0	5	4	48.44

Sodium Barbital, $C_8H_{11}N_2NaO_3$ - (continued)

d(Å)	Ι	hkl 20(°) ° λ - 1.540598A
1.8683 1.8589	2	2 2 5 48.7 ⁽ 3 3 2 48.96
1.8420	3 2 2	1 2 6 49.44
1.7985		2 4 4 50.72
1.7737	1	3 4 1 51.48
1.7584	1	3 3 3 51.96
1.7547	2	2 5 3 52.08
1.7410	1	1 3 6 52.52
1.7324	1	2 0 6 52.80
1.7270	1	1 6 3+ 52.98
1.7191	1	3 4 2 53.24
1.7150	2	2 1 6+ 53.38
1.6615	1	1 1 7+ 55.24
1.6489	2	2 6 2 55.70 3 4 3+ 56.06
1.6392	3	3 4 3+ 56.06
1.6159	1	1 6 4+ 56.94
1.6040	1	4 2 1+ 57.40
1.5784	1	3 5 2+ 58.42
1.5730	1	0 7 3 58.64

	Calculated	Pattern	(I	nte	grated)
d(A)	Ι	ŀ	ıkl	,	2Θ(°) λ - 1.540598Å
8.51	100	0	1	1	10.38
6.06	25	0	0	2	14.59
5.98	12	0 1	2	0	14.81
5.88	8 61	1	1	1 0	15.05 15.11
5.86	01	1	1	U	15.11
5.36	55	0	2	1	16.52
5.28	5	1	1	1	16.79
4.504		1	0	2	19.70
4.25		0	2	2 2	20.85
4.21	4 24	1	1	2	21.06
4.19	1 17	1	2	1	21.18
3.785		0	3	1	23.49
3.59		1	2	2	24.73
3.46		1	0	3	25.69
3.42	7 1	1	3	0	25.98
3.36	2 1	2	0	0	26.49
3.34		0	2	3	26.60
3.33		0	3	2	26.75
3.32		1	1	3	26.77
3.29		1	3	1	27.01
3.24	0 2	2	0	1	27.51
3.23		2	1	0	27.54
3.12		2	1	1	28.52
3.12		0	0	4	29.43
2.99		1	2	3	29.78
2.99	.	1	_	J	27.70

d(A)	I	ì	nkl		2Θ(°) ° λ - 1.540598A
2.988 2.984 2.930 2.901 2.855	5 4 3 3	0 1 2 0 2	4 3 2 4 1	0 2 0 1 2	29.88 29.92 30.48 30.80 31.30
2.848	2	2	2	1	31.38
2.838	18	0	3	3	31.50
2.764	1	1	0	4	32.36
2.693	3	1	1	4	33.24
2.664	7	1	4	1	33.62
2.638	4	2	2	2	33.95
2.614	9	1	3	3	34.27
2.509	6	1	2	4	35.76
2.490	2	1	4	2	36.05
2.403	8	0	4	3	37.39
2.3775	2	0	1	5	37.81
2.3726	2	2	2	3	37.89
2.3658	1	2	3	2	38.00
2+51	2	0	5	1	38.35
2.2711	6	1	3	4	39.65
2.2628	1	1	4	3	39.81
2.2521	1	1	5	0	40.00
2.2415	4	1	1	5	40.20
2.2237	1	0	5	2	40.53
2.2143	2	1	5	1	40.71
2.2040	2	3	0	1	40.91
2.2029	7	3	1	0	40.93
2.1685	2	2	3	3	41.61
2.1675	3	3	1	1	41.63
2.1113	1	1	5	2	42.80
2.1072	2	2	2	4	42.88
2.0720	1	0	3	5	43.65
2.0678	6	3	2	1	43.74
2.0576	2	0	5	3	43.97
2.0291	6	1	4	4	44.62
1.9801	4	1	3	5	45.79
1.9603	1	2	3	4	46.28
1.9534	2	3	3	0	46.45
1.9361	1	1	0	6	46.89
1.9344	2	3	1	3	46.93
1.8924	2	0	6	2	48.04
1.8866	3	1	6	1	48.20
1.8772	1	0	5	4	48.45
1.8686	2	2	2	5	48.69
1.8593	3	3	3	2	48.95
1.8418	3	1	2	6	49.45
1.7983	3	2	4	4	50.73
1.7736	1	3	4	1	51.48
1.7589	1	3	3	3	51.95
1.7550	2	2	5	3	52.07

Sodium Barbital, $C_8H_{11}N_2NaO_3$ - (continued)

d(Å)	I		hk	L	2Θ(°) λ - 1.540598A
1.7413	1	1	3	6	52.51
1.7325	1	2	0	6	52.80
1.7194	1	3	4	2	53.23
1.7146	2	2	1	6	53.39
1.6780	1	1	0	7	54.65
1.6617	1	1	1	7	55,23
1.6491	2	2	6	2	55.69
1.6390	1	2	5	4	56.07
1.6390	2	3	4	3	56.07
1.5728	1	0	7	3	58.65

$\Delta^9\text{-Tetrahydrocannabinolic Acid B, C}_{22}\mathrm{H}_{30}\mathrm{O}_4$

Δ	⁹ -Tetrahydrocannabi
Synonyms 1. delta (sup 9) - THC acid B 2. 6,6,9-trimethyl-3-pentyl-7 6H-dibenzo(b,d)pyran-1-ol	
Structure Orthorhombic, P2 ₁ 2 ₁ 2 ₁ (19), Z structure was refined by Rose Ottersen [1975].	= 4. The enqvist and
Atom positions All atoms were in general pos	itions 4(a).
Lattice constants a = 16.515(2) A b = 14.325(2) c = 8.744(1)	
(published values: a = 16.51 b = 14.324(2), c = 8.744(1) [Ottersen, 1975])	4(2) Å, Rosenqvist and
CD cell: $a = 14.325(2) \stackrel{\circ}{A}$, b c = 8.744(1). sp. gp. $P2_12_12_2$ c/b = 0.5295.	
Volume 0 2068.6 Å ³	
Density (calculated) 1.151 g/cm ³ (measured) 1.12 g/cm ³ [Rose Ottersen, 1975]	enqvist and
Thermal parameters For hydrogen: isotropic B of the sent of the	
Scattering factors H ⁰ [Stewart et al., 1965] C ⁰ , O ⁰ [Doyle and Turner, 196	58]
Scale factors (integrated interpretation $\gamma = 3.492 \times 10^{-3}$ I/I corundum (calculated) = 1 with hk ℓ = 110.	nsities)

	lculated	Pattern	(Pea	k l	neights)
d(A)	I		hkl		2Θ(°) λ - 1.540598Å
10.80	100	1	1	0	8.18
8.25	6	2	0	0	10.72
7.72	22	1	0	1	11.46
7.46	17	0	1	1	11.86
7.16	9	0	2	0	12.36
6.79	10	1	1	1	13.02
6.56	8	1	2	0	13.48
5.53	29	0	2	1+	16.00
5.13	4	3	1	0	17.26
4.65	3	3	0	1	19.06
4.59	8	2	2	1+	19.32
4.371	63	0	0	2	20.30
4.223	4	1	0	2	21.02
4.130	3	2	3	0+	21.50
4.052	43	1	1	2+	21.92
3.966	4	4		0	22.40
3.864	1	2	0	2	23.00
3.729	13	0	2	2+	23.84
3.639	11	1	2	2	24.44
3.582	1	0	4	0	24.84
3.399	4	2	2	2	26.20
3.329	4	3		2	26.76
3.314	3	4	2	1+	26.88
3.123	1	4		0	28.56
3.089	2.	3	2	2	28.88
2.855	4	0	1	3	31.30
2.840	2	3		1+	
2.704	2	4		0+	
2.664	1	1		3	33.62
2.585	2	4		1+	
2.541	1	3	5	0+	35.30
2.535	1	3		3	35.38
2.300		5		2+	
2.280		1	_	1+	
2.249		7		1	40.06
2.196	5 1	3	5	2	41.06
2.164		5		0+	
2.104		3		1+	
2.124		0		4+	
2.074		1		4	43.60
0.055	,	-	1	2.	44.02
2.055		7		2+	
2.026		2		4+	
1.989		8		1+	
1.953		3		4+	
1.934	9 1	2	. 7	1+	46.92
1.869	0 1	4	6	2+	48.68

 $\Delta^9\text{-Tetrahydrocannabinolic}$ Acid B, $\text{C}_{22}\text{H}_{30}\text{O}_4$ - (continued)

	Calculated	Patte	rn	(Int	tegrated)
d(A)	I		hl	r.l	2Θ(°) 。 λ - 1.540598A
10.82	100	1	1	0	8.16
8.26	6	2	0	0	10.71
7.73	22	1	0	1	11.44
7.46	16	0	1	1	11.85
7.16	9	0	2	0	12.35
6.80	10	1	1	1	13.01
6.57	7	1	2	0	13.46
5.54	19	0	2	1	15.98
5.54	11	2	1	1	15.99
5.14	4	3	1	0	17.24
4.66	3	3	0	1	19.04
4.60	6	2	2	1	19.28
4.59	4	1	3	0	19.33
4.430	4	3	1	1	20.03
4.372	69	0	0	2	20.30
4.226	4	1	0	2	21.00
4.134	2	2	3	0	21.48
4.062	16	1	3	1	21.86
4.054	35	1	1	2	21.91
3.967	3	4	1	0	22.39
3.864	1	2	0	2	23.00
3.737	2	2	3	1	23.79
3.732	10	0	2	2	23.83
3.731	3	2	1	2	23.83
3.640	12	1	2	2	24.43
3.613	1	4	1	1	24.62
3.581	1	0	4	0	24.84
3.424	1	3	0	2	26.01
3.401	4	2	2	2	26.18
3.330	4	3	1	2	26.75
3.314	1	0	4	1	26.88
3.311	2	4	2	1	26.91
3.123	2	4	3	0	28.56
3.089	2	3	2	2	28.88
2.856	4	0	1	3	31.29
2.839	2	3	4	1	31.48
2.705	2	4	4	0	33.09
2.700	1	0	2	3	33.16
2.664	1	1	2	3	33.61
2.584	1	4	4	1	34.68
2.535	1	3	1	3	35.38
2.2496	1	7	1	1	40.05
2.1972	1	3	5	2	41.05
2.1643	1	5	5	0	41.70
2.1427	1	1	1	4	42.14
2.1247	1	3	6	1	42.51
2.0742	1	1	2	4	43.60
2.0268	1	2	2	4	44.67
1.9897	1	8	1	1	45.55

Vinbarbital, Fo
Synonyms 1. 5-Ethyl-5(1-methyl-1-butenyl) barbituric acid
Structure Monoclinic, $P2_1/c$ (14), $Z = 4$. The structure was determined by Craven and Cusatis [1969].
Atom positions All atoms are in general positions 4(e). The reference was lacking data for H(221); it was omitted from these calculations.
Polymorphism Two polymorphs (melting points 129° and 106°) have been reported but they are very difficult to prepare from melt or solution [Craven and Cusatis, 1969].
Lattice constants a = 14.396(5) Å b = 6.822(3) c = 12.541(7) β = 107.43(3)°
a/b = 2.1102 c/b = 1.8383
(published values: $a = 14.395(5) \stackrel{\circ}{A}$, $b = 6.822(3)$, $c = 12.540(7)$, $\beta = 107° 26(2)'$ [Craven and Cusatis, 1969]
Volume 0 1175.1 A ³
Density (calculated) 1.268 g/cm ³
Thermal parameters Anisotropic for non-hydrogen atoms [Craven and Cusatis, 1969]. Overall B = 5.0 for hydrogen atoms.
Scattering factors C ⁰ , H ⁰ , N ⁰ , O ⁰ [International Tables, 1962]
Scale factors (integrated intensities) $\gamma = 2.068 \times 10^{-3}$ I/I corundum (calculated) = 0.799 for reflection with hk ℓ = 110.
Additional pattern 1. PDF card 9-555 [Parkes, E. B., South Western Forensic Science Lab., Westbury-on-Trym, Bristol, Eng.]

Bristol, Eng.]

Eng.) p. 202.

Craven, B. M. and Cusatis, C. (1969). Acta
Crystallogr. <u>B25</u>, 2291.

International <u>Tables for X-ray Crystallography</u>,

III (1962). (The Kynoch Press, Birmingham,

References

,	<u>-</u>					
		Calculated	Pattern	(Pea	ak h	neights)
	d(Å)	I		hkl		2Θ(°) λ - 1.540598A
	13.71 6.87 6.20 6.10 5.98	99 10 26 100 1 34	1 2 -1 1 0	0 0 0 1	0 0 2 0 2	6.44 12.88 14.28 14.50 14.80
	5.92 5.75 4.96 4.83 4.59	7 4 2 22 9 38	0 -1 1 2 -1	1 1 0 1	1 1 2 0 2	14.94 15.38 17.86 18.32 19.32
	4.49 4.30 4.18 4.01 3.91	8 5 8 17 5 1	0 -3 2 1 -3	1 0 1 1	2 2 1 2	19.72 20.60 21.20 22.12 22.70
	3.79 3.64 3.56 3.44 3.38	5 2 2 2 5 20	3 -3 -1 0 3	1 1 1 1	0 2 3 3+ 1	23.40 24.40 24.98 25.84 26.28
	3.30 3.28 3.20 3.12 3.05	1 4 2 17 5 19	1 0 3 -1 2	2 2 0 0 2	0 1 2 4+ 0+	26.92 27.16 27.84 28.54 29.20
	2.98 2.96 2.89 2.87 2.84	3 7 7 2 0 11	-1 0 3 2 -5	2 2 1 2 0	2 2 2 1 2+	29.88 30.14 30.84 31.14 31.48
	2.81 2.74 2.64 2.59 2.56	6 1 2 6 2 5	1 5 -1 0 3	2 0 2 2 2	2 0 3 3+ 1	31.80 32.58 33.90 34.58 34.90
	2.47 2.46 2.42 2.36 2.33	4 4 0 3 2 2	-4 3 4 5 -1	2 1 2 1 1	1+ 3 0 1 5+	36.32 36.44 37.12 38.06 38.52
	2.29 2.25 2.24 2.22 2.19	3 2 4 1 7 3	-4 0 1 -3 -5	2 1 3 2 2	3+ 5+ 0 4	39.22 39.98 40.16 40.48 41.06
	2.18 2.13 2.06 2.05 2.00	9 2 3 1 2 2	1 5 -1 -5 -1	3 2 0 1 2	1 0 6 5+ 5+	41.26 42.22 43.84 44.10 45.10

Vinbarbital, form I, $C_{11}H_{16}N_2O_3$ - (continued)

d(Å)	I	hkl 2Θ(°) ° λ - 1.540598A
2.005	2	-4 0 6 45.18
1.972	1	2 3 2+ 45.98
1.963	1	7 0 0+ 46.22
1.915	2	1 3 3+ 47.44
1.898	2	4 2 3+ 47.88
1.880	2	5 2 2 48.38
1.854	1	-7 1 4 + 49.10
1.782	1	- 2 2 6+ 51.22
1.722	1	0 2 6+ 53.16
1.710	1	- 6 2 5 53.56

Calculated Pattern (Integrated)

d(Å)	I	1	hkl		2Θ(°) ° λ - 1.540598A
13.73	96	1	0	0	6.43
6.87	10	2	0	0	12.88
6.21	19	-1	0	2	14.26
6.11	100	1	1	0	14.49
5.983	26	0	0	2	14.80
5.926	27	0	1	1	14.94
5.761	2	-1	1	1	15.37
4.967	23	1	0	2	17.84
4.840	40	2	1	0	18.32
4.591	37	-1	1	2	19.32
4.498	3	0	1	2	19.72
4.312	5	- 3	0	2	20.58
4.224	1	-2	1	2	21.02
4.190	19	2	1	1	21.19
4.016	1	1	1	2	22.12
3.915	7	-3	1	1	22.69
3.802	3	3	1	0	23.38
3.645	2	-3	1	2	24.40
3.564	2	-1	1	3	24.96
3.459	13	-4	0	2	25.74
3.457	4	-2	1	3	25.75
3.443	15	0	1	3	25.86
3.434	1	4	0	0	25.93
3.426	5	2	1	2	25.99
3.388	1	3	1	1	26.28
3.310	3	1	2	0	26.91
3.280	4	0	2	1	27.16
3.202	19	3	0	2	27.84
3.183	1	-4	1	1	28.01
3.174	1	-3	1	3	28.09
3.153	2	1	1	3	28.28
3.133	10	1	2	1	28.47
3.124	15	-1	0	4	28.55
3.067	4	4	1	0	29.09
3.055	8	2	2	0	29.21

d(Å)	I	hkl	2Θ(°) λ - 1.540598A
2.991 2.989 2.963 2.940 2.899	2 15 6 1	0 0 4 -1 2 2 0 2 2 -3 0 4 3 1 2	29.85 29.86 30.13 30.38 30.82
2.870 2.840 2.840 2.825 2.824	12 1 2 1	2 2 1 -1 1 4 -5 0 2 -2 1 4 -4 1 3	31.14 31.47 31.48 31.64 31.66
2.812	14	1 2 2	31.80
2.797	5	4 1 1	31.98
2.747	1	5 0 0	32.57
2.655	2	4 0 2	33.74
2.647	1	-5 1 1	33.84
2.643	6	-1 2 3	33.89
2.592	5	0 2 3	34.57
2.585	1	2 2 2	34.68
2.569	3	3 2 1	34.90
2.476	2	-4 2 1	36.26
2.471	2	-3 2 3 3 1 3 4 2 0 5 1 1 -1 1 5	36.32
2.463	3		36.45
2.420	3		37.12
2.362	2		38.06
2.336	1		38.50
2.335	1	3 2 2	38.53
2.258	1	0 1 5	39.89
2.254	1	5 0 2	39.98
2.243	1	1 3 0	40.16
2.227	4	-3 2 4	40.48
2.197	2	-5 2 1	41.06
2.186	1	1 3 1	41.27
2.139	2	5 2 0	42.21
2.063	1	-1 0 6	43.84
2.056	1	-6 1 4	44.01
2.052 2.009 2.008 2.005 1.962	2 2 1 1	-5 1 5 -1 2 5 2 2 4 -4 0 6 7 0 0	44.10 45.08 45.12 45.19 46.23
1.916	1	-4 2 5	47.42
1.916	1	1 3 3	47.42
1.914	1	0 1 6	47.46
1.899	2	4 2 3	47.87
1.880	2	5 2 2	48.37
1.854 1.782 1.722 1.710	1 1 1	-7 1 4 -2 2 6 0 2 6 -6 2 5	49.10 51.22 53.16 53.55

INORGANIC NAMES

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	Sec.	Page	V	ol. or Sec.	Page
Aluminum, Al	1	11	Ammonium aluminum selenate hydrate,	Sec.	Page
Aluminum antimony, AlSb	4	72	NH ₄ A1(SeO ₄) ₂ ·12H ₂ O	9m	6
Aluminum bismuth oxide, Al ₄ Bi ₂ O ₉	11m	5	Ammonium aluminum sulfate,		
Aluminum chloride, AlCl ₃	9m	61	NH ₄ A1(SO ₄) ₂	10m	5
Aluminum chloride hydrate			Ammonium aluminum sulfate hydrate		
(chloraluminite), AlCl ₃ ·6H ₂ O	7	3	(tschermigite), NH ₄ Al(SO ₄) ₂ ·12H ₂ O	6	3
Aluminum copper, Al ₄ Cu ₉	11m	79	Ammonium azide, NH_4N_3	9	4
Aluminum fluoride hydroxide silicate	,		Ammonium beryllium fluoride,		
topaz, $Al_2(F,OH)_2SiO_4$	lm	4	(NH ₄) ₂ BeF ₄	3m	5
Aluminum iron antimony oxide, bahian		0.7	Ammonium boron fluoride, NH ₄ BF ₄	3m	6
Al _{5.66} Fe _{0.09} Sb _{2.95} O ₁₆	16m	87	Ammonium bromide, NH ₄ Br	2	49
Aluminum iron oxide, AlFeO ₃	15m	7	Ammonium cadmium bromide, (NH ₄) ₄ CdBr ₆	15m	9
Aluminum lithium, Al ₄ Li ₉	10m	98 82	Ammonium cadmium chloride, NH ₄ CdCl ₃	5m	6
Aluminum nickel, AlNi	6m 12m	5	Ammonium cadmium sulfate, $(NH_4)_2Cd_2(SO_4)_3$	7m	5
Aluminum nitrate hydrate,	12111	J	Ammonium cadmium sulfate hydrate,	7111	J
A1(NO ₃) ₃ ·9H ₂ O	11m	6	$(NH_4)_2Cd(SO_4)_2 \cdot 6H_2O \cdot \cdot \cdot \cdot \cdot$	8m	5
Aluminum oxide (corundum), α -Al ₂ O ₃	9	3	Ammonium calcium sulfate,	0	Ŭ
Aluminum oxide hydrate (boehmite),		_	$(NH_4)_2Ca_2(SO_4)_3$	8m	7
α-Al ₂ O ₃ ·H ₂ O	3	38	Ammonium chlorate, NH ₄ ClO ₄		
Aluminum oxide hydrate, diaspore,			(orthorhombic)	7	6
β -Al ₂ O ₃ ·H ₂ O	3	41	Ammonium chloride (salammoniac),		
Aluminum phosphate, $Al(PO_3)_3$	2m	3	NH ₄ Cl	1	59
Aluminum phosphate (berlinite),			Ammonium chromium sulfate hydrate,		
AlPO ₄ (trigonal)	10	3	$NH_4Cr(SO_4)_2 \cdot 12H_2O$	6	7
Aluminum phosphate, AlPO ₄			Ammonium cobalt (II) chloride,		_
(orthorhombic)	10	4	NH ₄ CoCl ₃	6m	5
Aluminum plutonium, AlaPu	15m	77	Ammonium cobalt fluoride, NH ₄ CoF ₃	8m	9
Aluminum rhenium, Al Re	15m	79	Ammonium copper bromide hydrate,	7.0	
Aluminum rhenium, Al ₁₂ Re	15m 15m	80 82	(NH ₄) ₂ CuBr ₄ ·2H ₂ O	10m	6
Aluminum rhodium, AlRh	15m	83	Ammonium copper chloride, NH ₄ CuCl ₃	7m	7
Aluminum ruthenium, Al ₆ Ru	15m	84	Ammonium copper chloride hydrate,	12m	6
Aluminum samarium, AlSm ₂	15m	86	(NH ₄) ₂ CuCl ₄ ·2H ₂ O Ammonium copper fluoride, NH ₄ CuF ₃	11m	8
Aluminum samarium, AlSm ₃	15m	88	Ammonium gallium sulfate hydrate,	11	Ü
Aluminum samarium, Al ₂ Sm	15m	90	$NH_4Ga(SO_4)_2 \cdot 12H_2O$	6	9
Aluminum samarium, Al ₃ Sm	15m	91	Ammonium germanium fluoride,		
Aluminum silicate (mullite),			(NH ₄) ₂ GeF ₆	6	8
Al ₆ Si ₂ O ₁₃	3m	3	Ammonium hydrogen arsenate,		
Aluminum sulfate, $Al_2(SO_4)_3$	15m	8	NH ₄ H ₂ AsO ₄	16m	9
Aluminum technetium, Al ₆ Tc	15m	93	Ammonium hydrogen carbonate		
Aluminum terbium, Al ₂ Tb	15m	95	(teschemacherite), $(NH_4)HCO_3$	9	5
Aluminum terbium, Al ₂ Tb ₃	15m	96	Ammonium hydrogen phosphate,		
Aluminum thorium uranium, AlaThU	15m	98	NH ₄ H ₂ PO ₄	4	64
Aluminum tungsten, Al ₅ W, δ-phase	15m	100	Ammonium iodate, NH ₄ IO ₃	10m	7
Aluminum tungsten oxide, $Al_2(WO_4)_3$ Aluminum vanadium, $Al_{10}V$	11m 15m	7 102	Ammonium iodide, NH ₄ I	4	56
Aluminum vanadium, Al _{10.25} V	15m	104	Ammonium iridium chloride,	8	6
Aluminum vanadium, Al ₂₃ V ₄	15m	106	(NH ₄) ₂ IrCl ₆ Ammonium iron chloride hydrate,	8	U
Aluminum vanadium, $Al_{45}V_7$, α -phase	15m	108	(NH ₄) ₂ FeCl ₅ ·H ₂ O	14m	7
Aluminum ytterbium, Al ₂ Yb	15m	111	Ammonium iron fluoride, (NH ₄) ₃ FeF ₆	9m	9
Aluminum yttrium, Al ₃ Y	15m	112	Ammonium iron sulfate, NH ₄ Fe(SO ₄) ₂	10m	8
Ammonium aluminum fluoride,			Ammonium iron sulfate hydrate,		
(NH ₄) ₃ A1F ₆	9 m	5	$NH_4Fe(SO_4)_2 \cdot 12H_2O \dots$	6	10
			Ammonium lead chloride, (NH ₄) ₂ PbCl ₆	11m	10
			Ammonium magnesium aluminum fluoride,		
Further work on this program is			NH ₄ MgA1F ₆	10m	9
and it is anticipated that addition			Ammonium magnesium chromium oxide		
will be issued. Therefore, the cumu			hydrate, $(NH_4)_2Mg(CrO_4)_2 \cdot 6H_2O \dots$	8m	10
here is not necessarily the conc	luding i	ndex	Ammonium magnesium phosphate hydrate	2	/ 1
for the project.			(struvite), NH ₄ MgPO ₄ ·6H ₂ O	3m	41
m ~ Monograph 25. A mineral name in () indicates	a synthe	tic	Ammonium manganese chloride hydrate,	11m	11
sample.	bynene	310	(NH ₄) ₂ MnCl ₄ ·2H ₂ O	TIII	11

sample.

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Ammonium manganese(II) fluoride,			Antimony iron titanium oxide		
NH ₄ MnF ₃	5m	8	hydroxide, derbylite,		
Ammonium manganese sulfate,			SbFe ₄ Ti ₃ O ₁₃ (OH)	16m	89
$(NH_4)_2Mn_2(SO_4)_3$	7m	8	Antimony lanthanum, LaSb	4m	42
Ammonium manganese sulfate hydrate,	8 m	12	Antimony (III) ovide (separmentite)	4m	43
(NH ₄) ₂ Mn(SO ₄) ₂ ·6H ₂ O Ammonium mercury chloride, NH ₄ HgCl ₃	8m 8m	14	Antimony(III) oxide (senarmontite), Sb ₂ O ₃ (cubic)	3	31
Ammonium molybdenum oxide phosphate	O.III	Τ.	Antimony(III) oxide, valentinite,	3	31
hydrate, (NH ₄) ₃ (MoO ₃) ₁₂ PO ₄ ·4H ₂ O	8	10	Sb ₂ O ₃ (orthorhombic)	10	6
Ammonium nickel(II) chloride,			Antimony(IV) oxide (cervantite),		
NH ₄ NiCl ₃	6m	6	Sb ₂ 0 ₄	10	8
Ammonium nickel chromium oxide	0	1.0	Antimony(V) oxide, Sb ₂ O ₅	10	10
hydrate, (NH ₄) ₂ Ni(CrO ₄) ₂ ·6H ₂ O	8m	16	Antimony proceeds by Dr.Sh	16m 4m	14 43
Ammonium nitrate (nitrammite), NH ₄ NO ₃	7	4	Antimony praseodymium, PrSb Antimony scandium, SbSc	4m	44
Ammonium osmium bromide, (NH ₄) ₂ OsBr ₆	3	71	Antimony selenide, Sb ₂ Se ₃	3m	7
Ammonium osmium chloride,			Antimony silver sulfide, AgSbS ₂		
(NH ₄) ₂ 0sCl ₆	lm	6	(cubic)	5m	48
Ammonium palladium chloride,			Antimony silver sulfide (miargyrite),		
(NH ₄) ₂ PdCl ₄	6	6	AgSbS ₂ (monoclinic)	5m	49
Ammonium palladium chloride, (NH ₄) ₂ PdCl ₆	8	7	Antimony silver sulfide (pyrargyrite),	5 m	51
Ammonium platinum bromide,	J	,	Ag ₃ SbS ₃ (trigonal) Antimony silver telluride, AgSbTe ₂ .	3m	47
(NH ₄) ₂ PtBr ₆	9	6	Antimony (III) sulfide (stibnite),	5	.,
Ammonium platinum chloride,			Sb ₂ S ₃	5	6
(NH ₄) ₂ PtCl ₆	5	3	Antimony telluride, Sb ₂ Te ₃	3m	8
Ammonium potassium iron chloride			Antimony terbium, SbTb	5m	61
hydrate (kremersite),	1/	0	Antimony thorium, SbTh	4m	44
(NH ₄ ,K) ₂ FeCl ₅ ·H ₂ O	14m 9	8 7	Antimony tin ShSn	4m 16m	45 15
Ammonium rhenium oxide, NH ₄ ReO ₄ Ammonium selenium bromide,	,	,	Antimony tin, SbSn	4m	45
(NH ₄) ₂ SeBr ₆	8	4	Antimony yttrium, SbY	4m	46
Ammonium silicon fluoride			Arsenic, As	3	6
(cryptohalite), (NH ₄) ₂ SiF ₆	5	5	Arsenic cerium, AsCe	4m	51
Ammonium strontium chromium oxide,			Arsenic(III) iodide, AsI ₃	13m	7
(NH ₄) ₂ Sr(CrO ₄) ₂	14m	9	Arsenic oxide (arsenolite),	,	5.3
Ammonium strontium sulfate,	15m	11	As ₂ 0 ₃ (cubic)	1	51
$(NH_4)_2Sr(SO_4)_2$	13111	11	Arsenic oxíde, claudetite, As ₂ 0 ₃ (monoclinic)	3m	9
(NH ₄) ₂ SO ₄	9	8	Barium, Ba	4	7
Ammonium tellurium bromide,			Barium aluminum oxide, BaAl ₂ O ₄	5m	11
(NH ₄) ₂ TeBr ₆	8	5	Barium aluminum oxide, Ba ₃ Al ₂ O ₆	12m	7
Ammonium tellurium chloride,			Barium arsenate, $Ba_3(AsO_4)_2$	2m	6
(NH ₄) ₂ TeCl ₆	8	8	Barium borate, BaB ₄ O ₇	4m	6
Ammonium tin chloride, (NH ₄) ₂ SnCl ₆	5	4	Barium borate, high form, BaB ₂ O ₄	4m	4
Ammonium titanium fluoride, (NH ₄) ₂ TiF ₆	16m	10	Barium borate, BaB ₈ O ₁₃ Barium bromate hydrate,	7m	10
Ammonium vanadium oxide, NH ₄ VO ₃	8	9	Ba(BrO ₃) ₂ ·H ₂ O ····································	8m	19
Ammonium zinc chloride, (NH ₄) ₃ ZnCl ₅	15m	12	Barium bromide, BaBr ₂	10m	63
Ammonium zinc fluoride, NH ₄ ZnF ₃	8m	18	Barium bromide fluoride, BaBrF	10m	10
Ammonium zirconium fluoride,		- ,	Barium bromide hydrate, BaBr ₂ ·H ₂ O	3m	10
(NH ₄) ₃ ZrF ₇	6	14	Barium bromide hydrate, BaBr ₂ ·2H ₂ O	16m	16
Antimonic acid, $H_{14}Sb_{14}O_{21}(OH)_{42}$ Antimony, Sb	16m 3	13 14	Barium cadmium chloride hydrate,	15m	14
Antimony bromide, α -SbBr ₃	15m	13	BaCdCl ₄ ·4H ₂ O Barium calcium nitrate,	15m	14
Antimony cerium, CeSb	4m	40	Ba _{.25} Ca _{.75} (NO ₃) ₂	12m	38
Antimony cobalt, CoSb	15 m	121	Barium calcium nitrate,		
Antimony cobalt, CoSb ₂	15m	122	Ba _{.50} Ca _{.50} (NO ₃) ₂	12m	38
Antimony cobalt titanium, CoSbTi	15m	124	Barium calcium nitrate,	3.0	
Antimony duspressium Dush	15m	125	Ba _{.75} Ca _{.25} (NO ₃) ₂	12m	38
Antimony dysprosium, DySb Antimony erbium, ErSb	4m 4m	41 41	Barium calcium tungsten oxide, Ba ₂ CaWO ₆	Qm	10
Antimony(III) fluoride, SbF ₃	2m	4	Barium carbonate (witherite), BaCO ₃	9m	10
Antimony gadolinium, GdSb	4m	42	(orthorhombic)	2	54
Antimony gallium, GaSb	6	30	Barium carbonate, BaCO ₃ (cubic)		
Antimony gold (aurostibite), AuSb ₂	7	18	at 1075 °C	10	11
Antimony (III) indide Shi	4	73	Barium chlorate, Ba(ClO ₃) ₂	16m	17
Antimony(III) iodide, SbI ₃	6	16	65		

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Barium chlorate hydrate,			Beryllium calcium iron magnesium		
Ba(C10 ₄) ₂ ·3H ₂ O	2m	7	aluminum phosphate hydroxide		
Barium chlorate hydrate,			hydrate, roscherite (monoclinic),		
$Ba(C10_3)_2 \cdot H_2O$	8m	21	Be ₂ Ca(Fe _{.3} Mg _{.7}) ₂ Al _{.67} (PO ₄) ₃ (OH) ₃ ·2H ₂	20 16m	96
Barium chloride, BaCl ₂ , (cubic)	9 m	13	Beryllium calcium manganese		
Barium chloride, BaCl ₂ ,	0	11	aluminum iron phosphate hydroxide		
(orthorhombic)	9m	11	hydrate, roscherite (triclinic),		
Barium chloride fluoride, BaClF Barium chloride hydrate, BaCl ₂ ·2H ₂ O	10m 12m	11 9	Be ₄ Ca ₂ (Mn _{3.91} Mg _{.04} Ca _{.05})(Al _{.13} Fe _{.42} Mn _{.12})(PO ₄) ₆ (OH) ₄ ·6H ₂ O	16m	100
Barium chromium oxide,	12111	,	Beryllium calcium oxide,	TOIL	100
Ba ₃ (CrO ₄) ₂	15m	16	Be ₁₇ Ca ₁₂ O ₂₉	7m	89
Barium fluoride, BaF ₂	1	70	Beryllium chromium oxide, BeCr ₂ O ₄	10	12
Barium hydroxide phosphate,			Beryllium cobalt, BeCo	5m	62
Ba ₅ (OH)(PO ₄) ₃	11m	12	Beryllium germanium oxide, Be ₂ GeO ₄	10	13
Barium iodide, BaI ₂	10m	66	Beryllium lanthanum oxide, Be ₂ La ₂ O ₅	9m	65
Barium iodide hydrate, BaI ₂ ·2H ₂ O	16m	18	Beryllium niobium, Be ₂ Nb	7m	92
Barium lead chloride, BaPbCl ₄ Barium lead nitrate,	11m	13	Beryllium oxide (bromellite), BeO Beryllium palladium, BePd	1 5m	36 62
Ba . 33Pb . 67 (NO ₃) 2	12m	40	Beryllium silicate, phenakite,	Jiii	02
Barium lead nitrate,	+2	70	Be ₂ SiO ₄	8	11
Ba _{.67} Pb _{.33} (NO ₃) ₂	12m	40	Beryllium sulfate, BeSO ₄	15m	20
Barium manganese oxide,			Bismuth, Bi	3	20
$Ba(MnO_4)_2$	15m	17	Bismuth bromide oxide, BiOBr	8	14
Barium molybdenum oxide, BaMoO ₄	7	7	Bismuth cerium, BiCe	4m	46
Barium molybdenum oxide, Ba ₂ MoO ₅	12m	10	Bismuth chloride oxide (bismoclite),	,	F /
Barium nitrate (nitrobarite),	11	1/	BiOC1	4 /m	54
$Ba(NO_3)_2$	11m	14	Bismuth dysprosium, BiDy Bismuth erbium, BiEr	4m 4m	47 47
$Ba(NO_2)_2 \cdot H_2O \dots$	15m	18	Bismuth fluoride, BiF ₃	1m	7
Barium oxide, BaO	9m	63	Bismuth holmium, BiHo	4m	48
Barium oxide, BaO ₂	6	18	Bismuth(III) iodide, BiI ₃	6	20
Barium phosphate, Ba ₂ P ₂ O ₇ ,			Bismuth iodide oxide, BiOI	9	16
(high form)	16m	19	Bismuth lanthanum, BiLa	4m	48
Barium phosphate, Ba ₃ (PO ₄) ₂	12m	12	Bismuth neodymium, BiNd	4m	49
Barium selenide, BaSe	5m	61	Bismuth oxide (bismite), α -Bi ₂ O ₃	3m	16
Barium silicate, β-BaSiO ₃ Barium silicate (sanbornite),	13m	8	Bismuth phosphate, BiPO ₄	2	
β -BaSi ₂ O ₅	13m	10	(monoclinic)	3m 3m	11 13
Barium silicate, Ba ₂ SiO ₄	13m	12	Bismuth praseodymium, BiPr	4m	49
Barium silicate, Ba ₂ Si ₃ O ₈	13m	13	Bismuth sulfide (bismuthinite),		.,
Barium silicate, Ba ₃ SiO ₅	13m	15	Bi ₂ S ₃	5m	13
Barium silicate, Ba ₃ Si ₅ O ₁₃	13m	17	Bismuth telluride, BiTe	4m	50
Barium silicon fluoride, BaSiF ₆	4m	7	Bismuth telluride (tellurobis-		
Barium strontium nitrate,	10	/ 2	muthite), Bi ₂ Te ₃	3m	16
Ba _{.25} Sr _{.75} (NO ₃) ₂ Barium strontium nitrate,	12m	42	Bismuth vanadium oxide, low form,	2	1.6
Ba _50Sr _50(NO ₃) ₂	12m	42	BiVO ₄ (tetragonal)	3m	14
Barium strontium nitrate,			BiVO ₄ (monoclinic)	3m	14
Ba _{.75} Sr _{.25} (NO ₃) ₂	12m	42	Boron oxide, B_2O_3 , phase 1	10m	70
Barium sulfate (baryte), BaSO ₄	10m	12	Cadmium, Cd	3	10
Barium sulfide, BaS	7	8	Cadmium ammine chloride,		
Barium thiosulfate hydrate,			Cd(NH ₃) ₂ Cl ₂	10m	14
BaS ₂ O ₃ ·H ₂ O	16m	20	Cadmium borate, CdB ₄ O ₇	16m	24
Barium tin oxide, BaSnO ₃ Barium titanium oxide, BaTiO ₃	3m 3	11 45	Cadmium bromide, CdBr ₂	9 11m	17 15
Barium titanium silicate (fresnoite),		73	Cadmium bromide chloride, CdBrCl Cadmium carbonate (otavite), CdCO ₃	7	11
Ba ₂ TiSi ₂ O ₈	9m	14	Cadmium cerium, CdCe	5 m	63
Barium tungsten oxide, BaWO ₄	7	9	Cadmium chlorate hydrate,		
Barium tungsten oxide, Ba ₂ WO ₅	12m	14	Cd(C10 ₄) ₂ ·6H ₂ 0	3m	19
Barium vanadium oxide, Ba3(VO ₄) ₂	14m	10	Cadmium chloride, CdCl ₂	9	18
Barium zirconium oxide, BaZrO ₃	5	8	Cadmium chromium oxide, CdCr ₂ O ₄	5m	16
Beryllium, alpha, Be	9m	64	Cadmium copper, Cd ₈ Cu ₅	11m	81
Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄	9	10	Cadmium cyanide, Cd(CN) ₂	2m 10m	8 15
Beryllium aluminum silicate, beryl,		10	Cadmium fluoride, CdF ₂ Cadmium iron oxide, CdFe ₂ O ₄	9m	16
Be ₃ Al ₂ (SiO ₃) ₆	9	13	Cadmium lanthanum, CdLa	5m	63
			Cadmium manganese oxide, CdMn ₂ O ₄	10m	16
			Cadmium molybdenum oxide, CdMoO ₄	6	21

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Cadmium nitrate hydrate, Cd(NO ₃) ₂ ·4H ₂ O	7 m	93	Calcium gallium germanium əxide, Ca ₃ Ga ₂ (GeO ₄) ₃	10	18
Cadmium oxide, CdO	2	27	Calcium hydrogen phosphate hydrate,	10	10
Cadmium oxide, CdO (ref. standard)	8m	2	$Ca_8H_2(PO_4)_6 \cdot 5H_2O \dots$	13m	21
Cadmium phosphate, Cd ₂ P ₂ O ₇	16m	26	Calcium hydrogen phosphate sulfate		
Cadmium phosphate, $Cd_3(PO_4)_2$	-16m	27	hydrate, Ca ₂ HPO ₄ SO ₄ ·4H ₂ O	16m	109
Cadmium praseodymium, CdPr	5m	64	Calcium hydroxide (portlandite),		
Cadmium selenide (cadmoselite),	~	10	Ca(OH) ₂	1	58
CdSe (hexagonal)	7 13m	12 19	Calcium iodate (lautarite), Ca(IO ₃) ₂	14m	12
Cadmium silicate, Cd ₃ SiO ₅	13m	20	Calcium iodate hydrate,	14111	12
Cadmium sulfate, CdSO ₄	3m	20	Ca(IO ₃) ₂ ·6H ₂ O	14m	13
Cadmium sulfate hydrate,			Calcium iron germanium oxide,		
3CdSO ₄ · 8H ₂ O	6m	8	$Ca_3Fe_2(GeO_4)_3$	10	19
Cadmium sulfate hydrate, CdSO ₄ ·H ₂ O	6m	10	Calcium iron silicate (andradite),		
Cadmium sulfide (greenockite), CdS	4	15	Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22
Cadmium telluride, CdTe	3m	21 21	Calcium iron silicate		
Cadmium titanium oxide, CdTiO ₃ Cadmium tungsten oxide, CdWO ₄	15 m 2 m	8	hydroxide, julgoldite, Ca ₂ Fe ₃ Si ₃ O ₁₀ (OH,O) ₂ (OH) ₂	10m	72
Calcium, Ca	9m	68	Calcium lead nitrate,	10111	12
Calcium aluminum germanium oxide,	•		Ca _{.33} Pb _{.67} (NO ₃) ₂	12m	44
$Ca_3Al_2(GeO_4)_3$	10	15	Calcium lead nitrate,		
Calcium aluminum hydroxide,			Ca _{.67} Pb _{.33} (NO ₃) ₂	12m	44
Ca ₃ Al ₂ (OH) ₁₂	llm	16	Calcium magnesium silicate		
Calcium aluminum iron oxide	16.	0.0	(diopside), CaMg(SiO ₃) ₂	5m	17
(brownmillerite), Ca ₄ Al ₂ Fe ₂ O ₁₀	16m 5	28 10	Calcium molybdenum oxide	6	22
Calcium aluminum oxide, Ca ₃ Al ₂ O ₆ Calcium aluminum oxide (mayenite),	3	10	(powellite), $CaMoO_4$	7	14
Ca ₁₂ Al ₁₄ O ₃₃	9	20	Calcium oxide (lime), CaO	1	43
Calcium aluminum sulfate hydrate			Calcium oxide (lime), CaO		
(ettringite), Ca ₆ Al ₂ S ₃ O ₁₈ ·3lH ₂ O	8	3	(calculated pattern)	14m	49
Calcium borate, CaB ₂ O ₄	15m	136	Calcium oxide phosphate, Ca ₄ O(PO ₄) ₂	12m	17
Calcium borate hydrate,	16	7.0/	Calcium phosphate, β-Ca ₂ P ₂ O ₇	7m	95
hexahydroborite, Ca[B(OH) ₄] ₂ ·2H ₂ O	16m 16m	104 29	Calcium platinum oxide, Ca ₄ PtO ₆	10m	18 64
Calcium boride, CaB ₆	10m	70	Calcium selenide, CaSe	5m	04
Calcium bromide hydrate, CaBr ₂ ·6H ₂ O	8	15	Ca_33Sr_67(NO ₃) ₂	12m	46
Calcium carbonate (aragonite),			Calcium strontium nitrate,		
CaCO ₃ (orthorhombic)	3	53	Ca _{.67} Sr _{.33} (NO ₃) ₂	12m	46
Calcium carbonate (aragonite),			Calcium sulfate (anhydrite), CaSO ₄	4	65
CaCO ₃ (orthorhombic, calculated	2.4		Calcium sulfide (oldhamite), CaS	, 7	15
pattern)	14m	44	Calcium telluride, CaTe	4m	50
Calcium carbonate (calcite), CaCO ₃ (hexagonal)	2	51	Calcium titanium oxide (perovskite), CaTiO ₃	9m	17
Calcium chloride (hydrophilite),	2	J1	Calcium tungsten oxide, Ca ₃ WO ₆	9m	19
CaCl ₂	11m	18	Calcium tungsten oxide, scheelite,		
Calcium chloride fluoride, CaClF	10m	17	CaWO ₄	6	23
Calcium chloride hydrate,			Carbon, diamond, C	2	5
CaCl ₂ ·4H ₂ O	llm	73	Cerium arsenate, CeAsO ₄	4m	8
Calcium chloride hydrate	10	1.0	Cerium(III) chloride, CeCl ₃	lm	8
(antarcticite), CaCl ₂ ·6H ₂ O Calcium chromium germanium oxide,	12m	16	Cerium cobalt, CeCo ₂ Cerium cobalt, Ce ₂₄ Co ₁₁	13m 13m	50 51
$Ca_3Cr_2(GeO_4)_3$	10	16	Cerium copper, CeCu ₆	7m	99
Calcium chromium iron titanium			Cerium(III) fluoride, CeF ₃	8	17
oxide, loveringite, Ca _{.72} RE _{.33} (Y,			Cerium gallium, CeGa ₂	13m	54
Th,U,Pb).05Ti _{12.48} Fe _{3.38} Cr _{2.24}			Cerium magnesium, CeMg	5m	65
Mg.92Zr.58Al.39V.21Mn.04038	16m	106	Cerium magnesium, CeMg ₃	13m	56
Calcium chromium oxide (chromatite)		10	Cerium nickel, CeNi ₂	13m	58
CaCrO ₄ Calcium chromium oxide, Ca ₃ (CrO ₄) ₂	7 15m	13 22	Cerium niobium titanium oxide (aeschynite), CeNbTiO ₆	3m	24
Calcium chromium silicate	TOIL	22	Cerium nitride, CeN	4m	51
(uvarovite), Ca ₃ Cr ₂ (SiO ₄) ₃	10	17	Cerium(IV) oxide (cerianite), CeO ₂	1	56
Calcium fluoride (fluorite), CaF ₂	1	69	Cerium phosphide, CeP	4m	52
Calcium fluoride phosphate			Cerium thallium, CeTl	13m	59
(fluorapatite), Ca ₅ F(PO ₄) ₃	3m	22	Cerium thallium, CeTl ₃	13m	60
Calcium fluoride phosphate hydrate,	15	2/	Cerium (III) vanadium avida Cayo	13m	61
CaFPO ₃ ·2H ₂ O	15m	24	Cerium(III) vanadium oxide, CeVO ₄ Cerium zinc, CeZn	lm 5m	9 65
			167	7111	03

Cerium zinc, CcZna		\$7 - 1		Vo	1 00	
Cerium zinc, CeZn3		Vol. or Sec.	Page	Vo		Page
Cersium zinc, (c-Zng 14m 53 Cersium platinum bronide, CagPtEng 8 19 Cersium aluminum sulfate hydrate, Cash(Sng), 2128g 6 25 Cersium platinum flooride, CagPtEng 6 27 Cersium antimony fluoride, CasBFg 4m 9 Cersium silicum bronide, Cag-Berg 8 20 Cersium solitante bronide, Cag-Berg 7 7 7 7 7 7 7 7 7		500.	2 4 8 0			6 -
Cerium slice, Ce ₂ Za ₁ , 1-6m 55 Cerium platinum chloride, CsgPtCi ₀ 5 12 Cerium platinum sulfate hydrate, Cerium platinum chloride, CsgPti ₂ 6 27 Cerium slice hydrate, Cerium platinum fluoride, CsgPti ₃ 6 27 Cerium beryllium fluoride, CssPti ₃ 6 27 Cerium beryllium fluoride, CssPti ₃ 6 28 Cerium slice fluoride, CsgStPti ₃ 8 29 Cerium beron fluoride, CssPti ₃ 6 27 Cerium beryllium fluoride, CssPti ₃ 7 77 77 77 77 77 77 7	Cerium zinc, CeZn ₃	14m	50	Cesium osmium chloride, Cs ₂ OsCl ₆	2m	11
Cesium aluminum suifate hydrate, 6 25 Cesium platinum fluoride, CegFtFa 6 27 Cesium antimony fluoride, CSBFa 4m 9 Cesium silicon fluoride, CSBFa 5m 9m 9 Cesium silicon fluoride, CSBFa 5m 9m 9m 6m Cesium silicon fluoride, CSBFa 5m 3m 2c Cesium silicon fluoride, CSBFa 5m 2c Cesium cadmium chloride, CEGGTa 5m 2c Chromium, Cr 5m 2c Cesium chloride, CEGGTa 5m 2c Chromium chloride hydrate, CEGGTa 5m 2c Chromium chloride,						
Casium beryllium fluoride, Casber 4		14m	55			
Cesium antimony fluoride, CaSHF _a 59 66 Cesium striotony fluoride, CaSHF _a 58 22 Cesium strontium chloride, CaSTCH _a 59 24 Cesium bromate, CaSHF _a 59 24 Cesium bromate, CaSHF _a 59 24 Cesium thromate, CaSTCH _a 51 Cesium calcium the castCaSt _a 58 25 Cesium calcium the chloride, CaSCAST _a 58 25 Cesium calcium fluoride, CaSCAST _a 58 25 Chromate, CaSTCH _a 51 Cesium calcium fluoride, CaSCAST _a 58 25 Chromate, CaSTCH _a 51 Cesium calcium chloride, CaSCAST _a 58 25 Chromate, CaSTCH _a 51 Cesium chloride, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 25 Chromate, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 51 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 58 Chromate, CaSTCH _a 59 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 59 Cesium chloride, CaSCAST _a 58 Chromate, CaSTCH _a 59 Cesium chloride, CaSCAST _a 59 Chromate, CaSTCH _a 59 Chromate, CaSTCH _a 59 Cesium chloride, CaSCAST _a 59 Chromate, CaSTCH _a 59 Chromate, C		6	25			
Cesium beryllium filuoride, CabeF ₃ 9m 69 Cesium strontium chloride, CascL(3 6m 13 7 17 17 17 17 18 18 18						
Cesium boron fluoride, CsBF_						
Cesium bromate, CsBrOg.	_					
Cesium bromide, Csp. 3 49 Cesium tin chioride, Csp. 5 16	· ·	8	18		9	24
(hexagonal) (bm 20 CeS(S(SQ)2): 12H2Q 1 (cesium caldrium chloride, CsCaCl3 5m 19 Cesium calcitum chloride, CsCaCl3 7m 25 Cesium calcitum sulfatce, CsCaCl3 8m 25 Chromium chloride, CsCaCl3; 6HgQ 7m 25 Cesium calcitum sulfatce, CsCaCl3 8m 25 Chromium chloride, CsCaCl3; 6HgQ 16m 71 Cesium chlorate, CsGlQ3 8m 25 Chromium chloride, CsCaCl3; 6HgQ 16m 71 Cesium chlorate, CsGlQ3 8m 20 Chromium cobalt niobium, CoCrNa 15m 140 Cesium chloride, CsGlQ3 8m 20 Chromium cobalt niobium, CoCrNa 15m 140 Cesium chronium oxide, CsGlQ3 8m 20 Chromium cobalt niobium, CoCrNa 15m 140 Cesium chronium sulfate shydrate, 2 4d Chromium cobalt niobium, CoCrNa 15m 140 Cesium chronium sulfate, StGCl3 3m 25 Chromium plosphate, GCP3 5m 25 Cesium chronium sulfate, StGCl3 8m 21 Chromium plosphate, GCP3 <td>Cesium bromide, CsBr</td> <td>3</td> <td>49</td> <td></td> <td>5</td> <td>16</td>	Cesium bromide, CsBr	3	49		5	16
Cesium candmium chloride, CscGcl3	Cesium cadmium bromide, CsCdBr ₃			Cesium vanadium sulfate hydrate,		
Chexagonal		10m	20		lm	11
Chromium calcium chloride, CsCaIs		5 m	10		7	25
Cesium calcium fuloride, CsCaF3						
Cesium claim sulfate,						
Casia_(Sa_0)_3		Oili	23			
Cesium chloride, Cs2cCtl3		7 m	12			
Cesium chlorate, CsClO ₃ S 20 Co ₅ Cr ₁ ,Si ₆ Chromium Cobalt tantalum, CoCr ² 15m 142 (orthorhombic)		14m	58	· · · · · · · · · · · · · · · · · · ·		
Cesium chloride, CsCl 2		8	20	Co ₉ Cr ₁₅ Si ₆	14m	62
Cesium chloride, CsC 2				Chromium cobalt tantalum, CoCrTa		
Cesium chromium oxide, Cs ₂ CrO ₄ 3m 25 Chromium (III) fluoride hydrate, CsCr(So ₄) ₂ ·12H ₂ O						
CSCI (SQ ₄) ₂ -12H ₂ O					7m	108
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		3m	25		Em	25
Cesium cobalt (II) chloride, CSCOC14	and the same of th	ρ	21	_		
Cesium cobalt chloride, Cs_2CoLl ₄						
Cesium copper (II) chloride, CsCuCl ₃ 5m 22 Chromium phosphate, β-CrPO ₄ 9 26 Cesium copper sulfate hydrate, Cs ₂ Cu(SO ₄) ₂ ·6H ₂ O						
Cesium copper chloride, Cs2CuCl4 11m 20						
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		11m	20			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					15m	27
Cesium gallium sulfate hydrate, Cosium gallium sulfate hydrate, Cosium gallium sulfate hydrate, Cosium garmanium fluoride, Cs26eF6	$Cs_2Cu(SO_4)_2 \cdot 6H_2O \dots$	7m				
CSGa(SO ₄) ₂ ·12H ₂ O		3m	26			
Cesium germanium fluoride, Cs_2GeF_6 5 17 Cobalt aluminum oxide, $CoAl_2O_4$ 9 27 Cesium iodate, $CsIO_3$ 15m 26 Cobalt ammine iodide, $Co(MH_3)_6I_3$ 10m 83 26 Cesium iodide, CsI 4 47 Cobalt ammine iodide, $Co(MH_3)_6I_3$ 10m 26 Cesium iodide, CsI 3 50 Cobalt arsenide, $CoAs_2$ 4m 10 Cesium iron chloride hydrate, $Cs_2FeCl_5 \cdot H_2O$ 14m 14 Cobalt borate, $Co_3(BO_3)_2$ 12m 20 Cesium iron sulfate hydrate, $Cs_2FeCl_5 \cdot H_2O$ 14m 14 Cobalt borate, $Co_3(BO_3)_2$ 12m 20 Cesium iron sulfate hydrate, $Cs_2FeCo_3 \cdot I_2O$ 21 Cesium lead(II) chloride, $Cs_2FeCo_3 \cdot I_2O$ 22 Cesium lead fluoride, $Cs_2FeCo_3 \cdot I_2O$ 24 Cobalt chloride hydrate, $Co(2O_3 \cdot I_2O)$ 3m 28 (tetragonal) 5m 24 Cobalt chloride hydrate, $Co(2O_2 \cdot I_2O)$ 11m 22 Cesium lithium cobalt cyanide, $Cs_2O_3 \cdot I_2O$ 21 Cobalt chloride hydrate, $Co(2O_2 \cdot I_2O)$ 11m 23 Cesium lithium fluoride, $Cs_2FeCo_3 \cdot I_2O$ 21 Cobalt chloride hydrate, $Co(2O_2 \cdot I_2O)$ 12m 21 Cobalt chloride hydrate, $Co(2O_2 \cdot I_2O)$ 11m 22 Cobalt chloride hydrate, $Co(2O_2 \cdot I_2O)$ 11m 23 Cesium magnesium chromium oxide, $Cs_2O_3 \cdot I_2O$ 21 Cobalt copper tin, $Co_2O_2 \cdot I_2O$ 11m 23 Cesium magnesium chromium oxide, $Cs_2O_3 \cdot I_2O$ 25 Cobalt fluoride hydrate, $Co_2O_3 \cdot I_2O$ 13m 64 Csymga(CrO4)2-6H2O 8m 29 Cobalt fluoride hydrate, $Co_2O_3 \cdot I_2O$ 13m 64 Csymganese sulfate hydrate, $Cs_2O_3 \cdot I_2O$ 15m 15m 164 Cobalt gadolinium, $Co_2O_3 \cdot I_2O$ 11m 24 Cobalt gadolinium, $Co_2O_3 \cdot I_2O$ 11m 24 Cobalt gadolinium, $Co_3O_3 \cdot I_2O$ 11m 26 Cobalt gallium manganese, $Co_2O_3 \cdot I_2O$ 11m 27 Cesium manganese fluoride, $Cs_3O_3 \cdot I_2O$ 15m 22 Cobalt gallium manganese, $Co_2O_3 \cdot I_2O$ 13m 75 Cesium manganese sulfate hydrate, $Cs_2O_3 \cdot I_3O$ 15m 16 Cobalt gallium miobium, $Co_3O_3 \cdot I_3O$ 15m 16 Cobalt gallium miobium, $Co_3O_3 \cdot I_3O$ 15m 16 Cobalt gallium noibium, Co_3O_3		0	22			
Cesium iodate, CslO3						
Cesium iodide, CsI						
Cesium iodine bromide, CsI_2Br						
Cesium iodine chloride, CsĪCl2 3 50 Cobalt arsenide (skutterudite), 10 21 21 22 22 22 23 24 20 22 24 20 22 22 22		7 m			4m	10
Cs2FeCls'H2O 14m 14 Cobalt borate, Co3(BO3)2 12m 20 Cssium iron sulfate hydrate, Cobalt bromide hydrate, CoBr2'6H2O 12m 21 Cs2Fe(SO4)2'6H2O 7m 16 Cobalt (III) carbonate (sphaero-cobaltite), CoCO3 10 24 CsFe(SO4)2'12H2O 6 28 Cobalt chlorate hydrate, 3m 28 Cesium lead (II) chloride, CsPbCl3 6 28 Cobalt chlorate hydrate, 3m 28 Cesium lead fluoride, CsPbF3 8m 26 Cobalt chloride hydrate, CoCl2'2H2O 11m 23 Cesium lithium cobalt cyanide, Cobalt chloride hydrate, CoCl2'6H2O 11m 23 Cesium lithium fluoride, CsLiF2 7m 105 Cobalt chromium oxide, CoCr2O4 9m 21 CsliCo(CN)6 10m 79 Cobalt dysprosium, Co2Dy 13m 64 Cesium magnesium chromium oxide, CsLiF2 7m 105 Cobalt erbium, Co7Er2 13m 64 Cesium magnesium chromium oxide, Mydrate, Cs2Mg(CrO4)2'6H2O 8m 29 Cobalt fluoride, CoF2 11m 24 <		3	50	Cobalt arsenide (skutterudite),		
Comparison Com				CoAs ₃		
$ \begin{array}{c} \text{Cs}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O} & $		14m	14	Cobalt borate, $Co_3(BO_3)_2$		
Cesium iron sulfate hydrate, $CF_1(SO_4)_2 \cdot 12H_2O$	The state of the s	7	16		12m	21
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		/m	16		10	2/1
Cesium lead(II) chloride, CsPbCl3 (tetragonal)		6	28		10	24
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		Ŭ	20		3 m	28
Cesium lead fluoride, $CsPbF_3$ 8m 26 Cobalt chloride hydrate, $CoCl_2 \cdot 6H_2O$ 1lm 23 Cobalt chromium oxide, $CoCr_2O_4$ 9m 21 Cobalt chromium oxide, $CoCr_2O_4$ 9m 21 Cobalt chromium oxide, $CoCr_2O_4$ 9m 21 Cobalt copper tin, $CoCu_2Sn$ 14m 64 Cesium lithium fluoride, $CsLiF_2$ 7m 105 Cobalt dysprosium, Co_2Dy 13m 63 Cobalt erbium, Co_2Er 13m 64 Cs_Mg_2(CrO_4)_3 8m 27 Cobalt erbium, Co_2Er 13m 65 Cesium magnesium chromium oxide hydrate, $Cs_2Mg_2(CrO_4)_2 \cdot 6H_2O$ 8m 29 Cobalt fluoride, CoF_2 10m 85 hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$ 7m 18 Cobalt gadolinium, $CoGO_3$ 13m 68 Cs_Mg(SO_4)_2 \cdot 6H_2O 7m 18 Cobalt gadolinium, Co_2GO_3 13m 72 Cesium manganese fluoride, $CsMnF_3$ 10m 21 Cobalt gadolinium, Co_2GO_3 13m 72 Cobalt manganese sulfate hydrate, $Cs_2Mn(SO_4)_2 \cdot 6H_2O$ 7m 20 Cobalt gallium hafnium, Co_2GO_3 13m 75 Cesium mercury chloride, $CsMgCl_3$ 7m 20 Cobalt gallium manganese, Co_2GaMn 13m 75 Cesium nickel Sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 20 Cobalt gallium niobium, Co_2GaMn 15m 144 Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 23 Cobalt gallium niobium, Co_2GaMn 15m 144 Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 23 Cobalt gallium niobium, Co_2GaMn 15m 144 Cesium nitrate, $CsNO_3$ 9 25 Cobalt gallium tantalum, Co_2GaMn 15m 146 Cesium nitrate, $CsNO_3$ 9 25 Cobalt gallium tantalum, Co_2GaMn 15m 146		5m	24			22
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		8m	26		11m	
Cesium lithium fluoride, $CsLiF_2$ $7m$ 105 Cobalt dysprosium, Co_2Dy $13m$ 63 Cesium magnesium chromium oxide, $Cs_2Mg_2(CrO_4)_3$ $8m$ 27 Cobalt erbium, Co_2Er $13m$ 65 Cesium magnesium chromium oxide $Co_2Mg_2(CrO_4)_2 \cdot 6H_2O$ $8m$ 29 Cobalt fluoride, CoF_2 $10m$ 85 hydrate, $Cs_2Mg(CrO_4)_2 \cdot 6H_2O$ $8m$ 29 Cobalt fluoride hydrate, $CoF_2 \cdot 4H_2O$ 11m 24 Cesium magnesium sulfate hydrate, $Cs_2Mg(SO_4)_2 \cdot 6H_2O$ $7m$ 18 Cobalt gadolinium, Co_2Gd $13m$ 68 $Cs_2Mg(SO_4)_2 \cdot 6H_2O$ $7m$ 18 Cobalt gadolinium, Co_2Gd $13m$ 71 Cesium manganese sulfate hydrate, $Co_2Mn(SO_4)_2 \cdot 6H_2O$ $7m$ 20 Cobalt gallium hafnium, Co_2Gd $13m$ 72 Cesium mercury chloride, Cs_1MgCl_3 $7m$ 20 Cobalt gallium manganese, Co_2GaMn 13m 75 Cesium nickel(II) chloride, Cs_1MgCl_3 $7m$ 22 Cobalt gallium niobium, Co_2GaMn 13m 75 Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium niobium, Co_2GaNb 14m 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium niobium, Co_2GaNb 14m 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium niobium, Co_2GaNb 14m 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium niobium, Co_2GaNb 15m 144 Cesium nitrate, $Cs_1Mg_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium tantalum, $Co_2GaNb \cdot 14m$ 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium tantalum, $Co_2GaNb \cdot 14m$ 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium tantalum, $Co_2GaNb \cdot 14m$ 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $7m$ 23 Cobalt gallium tantalum, $Co_2GaNb \cdot 14m$ 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ $Cos_2OSBr_6 \cdot 14m$ 67 $Cos_2OSBr_6 \cdot 14m$ 68 $Cos_2OSBr_6 \cdot 14m$ 69 C	Cesium lithium cobalt cyanide,			Cobalt chromium oxide, CoCr ₂ O ₄	9m	
Cesium magnesium chromium oxide, $Cobalt erbium$, Co_2Er						
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		7m	105			
Cesium magnesium chromium oxide hydrate, $Co_2Mg(CrO_4)_2 \cdot 6H_2O$		0	0.7			
hydrate, $\operatorname{Cs_2Mg}(\operatorname{CrO_4})_2 \cdot \operatorname{6H_2O} \dots$ 8m 29 Cobalt fluoride hydrate, $\operatorname{CoF_2} \cdot \operatorname{4H_2O} $ 11m 24 Cesium magnesium sulfate hydrate, $\operatorname{Cs_2Mg}(\operatorname{SO_4})_2 \cdot \operatorname{6H_2O} \dots$ 7m 18 Cobalt gadolinium, $\operatorname{Co_2Gd} \dots$ 13m 71 Cesium manganese fluoride, $\operatorname{CsMnF_3} = \operatorname{Cobalt} = Cob$		OIII	21			
Cesium magnesium sulfate hydrate, $Cobalt gadolinium, Cocd_3 \dots 13m 68$ $Cocosium manganese fluoride, CsMnF_3 10m 21 Cobalt gadolinium, Cococosium manganese sulfate hydrate, Cocococosium manganese sulfate hydrate, Cococococococosium manganese sulfate hydrate, Cocococococococococococococococococococ$		8m	29			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		Oili			_	
Cesium manganese fluoride, $CsMnF_3$ 10m 21 Cobalt gadolinium, Co_7Gd_2 13m 72 Cobalt gallium hafnium, Co_2GaHf 14m 65 $Cs_2Mn(SO_4)_2 \cdot 6H_2O$ 7m 20 Cobalt gallium manganese, Co_2GaMn 13m 75 Cesium mercury chloride, $CsHgCl_3$ 7m 22 Cobalt gallium niobium, $Co_1.5Ga_0.5Nb$ 15m 144 Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 23 Cobalt gallium niobium, Co_2GaNb 14m 66 Cobalt gallium niobium, Co_2GaNb 14m 66 Cobalt gallium niobium, Co_2GaNb 14m 66 Cobalt gallium oxide, $CoGa_2O_4$ 10 27 Cesium nitrate, $CsNO_3$ 9 25 Cobalt gallium tantalum, $Co_1.5Ga_0.5Ta$ 15m 146		7m	18		13m	71
Cesium manganese sulfate hydrate, $Cobalt gallium hafnium, Co_2GaHf \dots 14m 65$ $Cobalt gallium manganese, Co_2GaMn 13m 75$ Cesium mercury chloride, $Cobalt gallium manganese, Co_2GaMn 13m 75$ Cesium nickel(II) chloride, $Cobalt gallium niobium, Cobalt gallium niobium, C$					13m	
Cesium nickel (II) chloride, $CsHgCl_3$ 7m 22 Cobalt gallium niobium, $Co_1 \cdot 5Ga_0 \cdot 5Nb$ 15m 144 Cesium nickel sulfate hydrate, $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 23 Cobalt gallium niobium, Co_2GaNb 14m 66 Cesium nitrate, $CsNO_3$ 9 25 Cobalt gallium tantalum, $Co_1 \cdot 5Ga_0 \cdot 5Nb$ 10 27 Cesium osmium(1V) bromide, Cs_2OsBr_6 2m 10 $Co_1 \cdot 5Ga_0 \cdot 5Ta$ 15m 146						
Cesium nickel(II) chloride, CsNiCl $_3$ 6m 12 Co $_1$,5Ga $_0$,5Nb		7 m			13m	75
Cesium nickel sulfate hydrate, Cobalt gallium niobium, Co_2GaNb 14m 66 $Cs_2Ni(SO_4)_2 \cdot 6H_2O$ 7m 23 Cobalt gallium oxide, $CoGa_2O_4$ 10 27 Cesium nitrate, $CsNO_3$ 9 25 Cobalt gallium tantalum, Cesium osmium(1V) bromide, Cs_2OsBr_6 2m 10 $Co_{1.5}Ga_{0.5}Ta$ 15m 146					15	17.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		6m	12			
Cesium nitrate, $CsNO_3$		7m	23			
Cesium osmium($1V$) bromide, Cs_2OsBr_6 2m 10 $Co_{1.5}Ga_{0.5}Ta$						~ '
168					15m	146
	, , ,			168		

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Cobalt gallium tantalum, Co ₂ GaTa	13m	76	Cobalt ruthenium sulfide, Co ₈ RuS ₈	14m	100
Cobalt gallium titanium, Co ₂ GaTi	13m	77	Cobalt samarium, Co ₂ Sm	15m	173
Cobalt gallium vanadium, Co ₂ GaV	13m	78	Cobalt samarium, Co ₅ Sm	13m	90
Cobalt germanium, Co ₃ Ge ₂	14m	67	Cobalt silicate, Co ₂ SiO ₄		
Cobalt germanium, Co ₅ Ge ₇	15m	148	(orthorhombic)	4m	11
Cobalt germanium hafnium,	1 /m	69	Cobalt silicon fluoride hydrate,	2	2.7
Co ₁₆ Ge ₇ Hf ₆ Cobalt germanium manganese,	14m	09	$CoSiF_6 \cdot 6H_2O$	3m 2m	27 14
Co ₂ GeMn	13m	79	Cobalt tantalum silicide,	2111	14
Cobalt germanium niobium,			Co ₁₆ Ta ₆ Si ₇	14m	102
Co _{1.5} Ge _{0.5} Nb	15m	150	Cobalt thorium, Co ₁₇ Th ₂	12m	64
Cobalt germanium niobium,			Cobalt tin, Co_3Sn_2	13m	92
Co ₁₆ Ge ₇ Nb ₆	14m	71	Cobalt tin oxide, Co ₂ SnO ₄	15m	30
Cobalt germanium oxide, Co ₂ GeO ₄	10	27	Cobalt tin vanadium, Co ₂ SnV	15m	174
Cobalt germanium tantalum, Co _{1.5} Ge _{0.5} Ta	15m	152	Cobalt tin zirconium, Co ₂ SnZr Cobalt titanium oxide, CoTiO ₃	15 m 4 m	175 13
Cobalt germanium tantalum,	10111	132	Cobalt titanium silicide,	7111	1.5
Co ₁₆ Ge ₇ Ta ₆	14m	73	Co ₁₆ Ti ₆ Si ₇	14m	104
Cobalt germanium titanium, Co ₂ GeTi	13m	80	Cobalt tungsten oxide, CoWO4	4m	13
Cobalt hafnium tin, Co ₂ HfSn	14m	75	Cobalt vanadium silicide, Co ₂ VSi	15m	176
Cobalt holmium, Co ₂ Ho	14m	76	Copper, Cu	1	15
Cobalt holmium, Co _{9.2} Ho ₁₂	15m	154	Copper ammine selenate,	1.0	0.7
Cobalt indium Coln	15m 13m	29 81	Cu(NH ₃) ₄ SeO ₄	10m	87
Cobalt indium, CoIn ₃	4m	52	Copper ammine sulfate hydrate, Cu(NH ₃) ₄ SO ₄ ·H ₂ O	10m	90
Cobalt iron arsenide		32	Copper antimony oxide, CuSb ₂ O ₆	5 m	27
(safflorite), CoFeAs ₄	10	28	Copper arsenate (trippkeite),	•	
Cobalt iron oxide, CoFe ₂ O ₄	9m	22	CuAs ₂ O ₄	16m	120
Cobalt iron sulfide, Co ₈ FeS ₈	14m	77	Copper(I) bromide, CuBr	4	36
Cobalt iron vanadium,	- 4		Copper(I) chloride (nantokite),		
Co _{4.35} Fe _{13.47} V _{12.18}	14m	79	CuCl	4	35
Cobalt lutetium Co.Iv	13m 13m	83 86	Copper fluoride hydrate, CuF ₂ ·2H ₂ 0	11m	25
Cobalt lutetium, Co ₂ Lu	15m	156	Copper hydrogen phosphite hydrate, CuHPO ₃ ·2H ₂ O	11m	83
Cobalt manganese silicide, Co ₂ MnSi	14m	81	Copper hydroxide carbonate,	11111	0.5
Cobalt mercury thiocyanate,	2	01	azurite, Cu ₃ (OH) ₂ (CO ₃) ₂	10	30
Co[Hg(CNS) ₄]	2m	13	Copper hydroxide carbonate		
Cobalt molybdenum, Co ₂ Mo	14m	82	(malachite), $Cu_2(OH)_2CO_3$	10	31
Cobalt molybdenum, Co ₂ Mo ₃	15m	158	Copper(I) iodide (marshite), CuI	4	38
Cobalt molybdenum, Co ₇ Mo ₆	15m	160	Copper lead hydroxide sulfate,	16m	34
Cobalt molybdenum silicide, Co ₃ Mo ₂ Si	15m	162	linarite, CuPb(OH) ₂ (SO ₄) Copper(I) oxide (cuprite), Cu ₂ O	2	23
Cobalt neodymium, Co ₂ Nd	13m	87	Copper(II) oxide (tenorite), CuO	1	49
Cobalt nickel tin,		- '	Copper phosphate, Cu(PO ₃) ₂	14m	15
Co.75Ni.75Sn.75	13m	88	Copper phosphate, α -Cu ₂ P ₂ O ₇	7 m	113
Cobalt niobium silicide, Co ₃ Nb ₄ Si ₇	15m	164	Copper sulfate (chalcocyanite),		
Cobalt midwate budgets	15m	166	CuSO ₄	3m	29
Cobalt nitrate hydrate, α-Co(NO ₃) ₂ ·6H ₂ O	12m	22	Copper(II) sulfide (covellite), CuS Copper uranium oxide, CuUO ₄	4 10m	13 93
Cobalt(II) oxide, CoO	9	28	Dichlorotetraaquochromium (III)	TOIL	93
Cobalt(II,III) oxide, Co ₃ O ₄	9	29	chloride dihydrate, $[Cr(H_2O)_4Cl_2]$		
Cobalt phosphate, Co(PO ₃) ₂	13m	23	C1 · 2H ₂ O	16m	31
Cobalt phosphide, CoP	14m	83	Dysprosium arsenate, DyAsO ₄	3m	30
Cobalt phosphide, CoP ₃	14m	85	Dysprosium arsenide, DyAs	4m	53
Cobalt platinum, CoPt (disordered)	15m	167	Dysprosium gallium oxide,	0	3.5
Cobalt platinum, CoPt (ordered)	15m	168	Dy ₃ Ga ₅ O ₁₂	2m	15
Cobalt platinum, CoPt ₃ (disordered)	15m	169	Dysprosium gold, DyAu	5m 4m	66 53
Cobalt platinum, CoPt ₃ (ordered)	15m	170	Dysprosium oxide, Dy ₂ O ₃		30
Cobalt plutonium, CoPu ₂	14m	87	Dysprosium silver, DyAg	5m	66
Cobalt plutonium, CoPu ₃	15m	171	Dysprosium telluride, DyTe	4m	54
Cobalt plutonium, CoPu ₆	14m	89	Dysprosium vanadium oxide, ${ m DyVO_4}$	4m	15
Cobalt plutonium, Co ₂ Pu	14m	91	Erbium arsenate, ErAsO ₄	3m	31
Cobalt plutonium, Co ₃ Pu	14m	92	Erbium arsenide, ErAs	4m	54
Cobalt plutonium, Co ₁₇ Pu ₂ Cobalt praseodymium, Co ₂ Pr	14m 14m	94 97	Erbium gallium oxide, Er ₃ Ga ₅ O ₁₂ Erbium manganese oxide, ErMnO ₃		12 16
Cobalt rhodium sulfide, Co ₈ RhS ₈	14m	98	Erbium nitride, ErN	4m	55
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Erbium oxide, Er ₂ O ₃	8	25	Hydrogen amidosulfate, H ₂ NSO ₃ H	7	54
Erbium phosphate, ErPO ₄	9	31	Hydrogen arsenate, H ₅ As ₃ O ₁₀	7m	84
Erbium silver, ErAg	5m	67	Hydrogen borate, β -HBO ₂ (monoclinic)	9m	71
Erbium telluride, ErTe	4m	55	Hydrogen borate (metaborite),		
Erbium vanadium oxide, ErVO ₄	5m	29	HBO ₂ (cubic)	4m	27
Europium arsenate, EuAsO ₄	3m	32	Hydrogen iodate, HIO ₃	5	28
Europium(III) chloride, EuCl ₃	lm	13	Hydrogen iodate, HI ₃ 0 ₈	8m	104
Europium chloride oxide, EuClo	lm	13	Hydrogen phosphate hydrate,	7.0	
Europium gallium oxide,	2	17	H ₃ PO ₄ ·0.5H ₂ O	12m	56
Eu ₃ Ga ₅ O ₁₂	2m	17	Hydrogen tellurate, H ₆ TeO ₆	12m	34
Europium nitride, EuN	4m 4m	56 56	Indium, In	3	12 35
Europium phosphate EuPO	11m	26	Indium arsenide, InAs	3m 5	26
Europium phosphate, EuPO ₄ Europium(III) vanadium oxide, EuVO ₄	4m	16	Indium oxide, In ₂ O ₃ Indium phosphate, InPO ₄	8	29
Gadolinium arsenate, GdAsO ₄	4m	17	Indium sulfide, In ₂ S ₃	11m	30
Gadolinium arsenide, GdAs	4m	57	Iodine, I ₂	3	16
Gadolinium chloride hydrate,		0,	Iridium, Ir	4	9
GdCl ₃ ·6H ₂ O	7m	118	Iridium niobium, IrNb ₃	6m	19
Gadolinium chloride oxide, GdClO	1m	17	Iridium oxide, IrO ₂	4m	19
Gadolinium fluoride, GdF ₃	lm	14	Iridium titanium, ĪrTi ₃	6m	20
Gadolinium gallium oxide,			Iridium vanadium, IrV ₃	6m	21
Gd ₃ Ga ₅ O ₁₂	2m	18	Iron, α-Fe	4	3
Gadolinium indium, GdIn	5m	67	Iron arsenide, FeAs	lm	19
Gadolinium nitride, GdN	4m	57	Iron arsenide (loellingite), FeAs ₂	10	34
Gadolinium oxide, Gd ₂ O ₃	lm	16	Iron bromide, FeBr ₂	4m	59
Gadolinium silver, GdAg	6m	87	Iron carbonate, siderite, FeCO ₃	15m	32
Gadolinium titanium oxide, Gd ₂ TiO ₅	8m	32	Iron chloride hydrate, FeCl ₂ ·2H ₂ O	llm	32
Gadolinium vanadium oxide, GdVO ₄	5m	30	Iron fluoride hydrate, FeF ₂ ·4H ₂ O	11m	90
Gallium, Ga	2	9	Iron hydroxide sulfate hydrate,	10m	95
Gallium arsenide, GaAs	3m 2m	33 22	butlerite, Fe(OH)SO ₄ ·2H ₂ O	10m 4m	60
Gallium magnesium, Ga ₂ Mg	12m	48	<pre>Iron iodide, FeI₂ Iron(II,III) oxide (magnetite),</pre>	7111	00
Gallium magnesium, Ga ₅ Mg ₂	12m	51	Fe ₃ 0 ₄	5m	31
Gallium neodymium oxide, Ga ₅ Nd ₃ O ₁₂	lm	34	Iron phosphate, FePO ₄	15m	33
Gallium oxide, α-Ga ₂ O ₃	4	25	Iron phosphate hydrate (vivianite),		
Gallium phosphate (α-quartz type),			Fe ₃ (PO ₄) ₂ ·8H ₂ O	16m	38
GaPO ₄	8	27	Iron sulfate, $Fe_2(SO_4)_3$	16m	39
Gallium phosphate hydrate,			Iron sulfate hydrate (melanterite),		
GaPO ₄ ·2H ₂ O	8m	34	FeSO ₄ •7H ₂ O	8m	38
Gallium samarium oxide, Ga ₅ Sm ₃ O ₁₂	lm	42	Iron sulfide (pyrite), FeS ₂	5	29
Gallium ytterbium oxide, Ga ₅ Yb ₃ O ₁₂	lm	49	Iron thorium, Fe ₁₇ Th ₂	12m	67
Gallium yttrium oxide, $Ga_5Y_3O_{12}$	lm	50	Iron titanium oxide (ilmenite),		
Germanium, Ge	,1	18	FeTiO ₃	15m	34
Germanium iodide, GeI ₂	4m	58	Lanthanum arsenate, LaAsO ₄	3m	36
Germanium (IV) iodide, GeI ₄	5	25	Lanthanum arsenide, LaAs	4m	60 20
Germanium oxide, GeO ₂ (hexagonal) (low form)	1	51	Lanthanum borate, LaBO ₃ Lanthanum chloride, LaCl ₃	lm lm	20
Germanium oxide, GeO ₂	-	31	Lanthanum chloride oxide, LaClO	7	22
(tetragonal) (high form)	8	28	Lanthanum fluoride, LaF ₃	7	21
Gold, Au	1	33	Lanthanum magnesium, LaMg	5m	69
Gold chloride, AuCl	16m	37	Lanthanum niobium titanium oxide,	J	
Gold(I) cyanide, AuCN	10	33	LaNbTiO ₆	3m	37
Gold holmium, AuHo	5m	68	Lanthanum nitrate hydrate,		
Gold magnesium, AuMg	6m	83	La(NO ₃) ₃ ·6H ₂ O	8m	40
Gold niobium, AuNb ₃	6m	16	Lanthanum nitride, LaN	4m	61
Gold potassium cyanide, $AuK(CN)_2$	8m	36	Lanthanum oxide, La ₂ O ₃	3	33
Gold tin, AuSn	7	19	Lanthanum phosphide, LaP	5m	69
Gold titanium, AuTi ₃	6m	17	Lanthanum selenide, LaSe	4m	61
Gold vanadium, AuV ₃	6m	18	Lanthanum titanium oxide, La ₂ Ti ₂ O ₇	15m	35
Hafnium, Hf	3	18	Lanthanum zinc, LaZn	5m	70
Holmium arsenate, HoAsO ₄	3m	34	Lead, Pb	1	34
Holmium fluoride, HoF ₃		23	Lead borate, PbB ₄ O ₇	4m	19
Holmium nitride, HoN	4m	58	Lead bromide, PbBr ₂	11m	47
Holmium oxide, Ho ₂ O ₃	,	32	Lead bromide chloride, PbBrCl	11m 10m	33 25
Holmium selenide, HoSe	4m 5m	59 68	Lead bromide fluoride, PbBrF	10m 16m	40
Holmium silver, HoAg	5m 4m	18	Lead bromide hydroxide, PbBr(OH) Lead bromide oxide, Pb ₃ O ₂ Br ₂	5m	32
mornium vanadrum oxide, novo4	7111		170	Jiii	J.

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Lead carbonate (cerussite), PbCO ₃ Lead chloride (cotunnite), PbCl ₂	2 12m	56 23	Lithium phosphate, low form (lithiophosphate), Li ₃ PO ₄	4m	21
Lead chloride fluoride (matlockite), PbClF	13m	25	Lithium phosphate, high form, Li ₃ PO ₄	3m	39
Lead chromium oxide, Pb ₂ CrO ₅	14m	16	Lithium potassium sulfate, KLiSO ₄	3m	43
Lead fluoride, α-PbF ₂			Lithium rubidium fluoride, LiRbF2	7m	128
(orthorhombic)	5	31	Lithium selenide, Li ₂ Se	10m	100
Lead fluoride, β-PbF ₂ (cubic)	5	33	Lithium silicate, Li ₂ SiO ₃	14m	19
Lead fluoride iodide, PbFI Lead hydrogen arsenate (schultenite)		26	Lithium silver bromide, Li _{.2} Ag _{.8} Br	12m	55
PbHAsO ₄	14m	18	Lithium silver bromide,	1.0	
Lead hydrogen phosphate, PbHPO ₄ Lead hydroxide phosphate,	15m	37	Li. ₄ Ag. ₆ Br Lithium silver bromide,	12m	55
Pb ₅ OH(PO ₄) ₃	8 5	33 34	Li ₆ Ag ₄ Br	12m	55 ⁻
Lead(II) iodide, PbI ₂ Lead molybdenum oxide (wulfenite),	J	34	Lithium silver bromide, Li_8Ag_2Br	12m	55
PbMoO ₄	7	23	Lithium sodium aluminum fluoride,		00
Lead nitrate, Pb(NO ₃) ₂	5	36	cryolithionite, Li ₃ Na ₃ Al ₂ F ₁₂	9m	23
Lead oxide (litharge), PbO (red,	•	0.0	Lithium sodium sulfate, LiNaSO ₄	6m	24
tetragonal)	2	30	Lithium sulfate, Li ₂ SO ₄	6m	26
Lead oxide (massicot), PbO (yellow, orthorhombic)	2	32	Lithium sulfate hydrate, Li ₂ SO ₄ ·H ₂ O	4m	22
Lead(II,III) oxide (minium), Pb ₃ O ₄	8	32	Lithium sulfide, Li ₂ S	10m	101
Lead oxide sulfate, Pb505S04	10m	27	Lithium tantalum oxide, LiTaO3	14m	20
Lead selenide (clausthalite), PbSe	5	38	Lithium telluride, Li ₂ Te	10m	102
Lead strontium nitrate,			Lithium tin oxide, Li ₂ SnO ₃	16m	45
Pb ₃₃ Sr ₆₇ (NO ₃) ₂	12m	53	Lithium tungsten oxide, Li ₂ WO ₄	1	25
Lead strontium nitrate, Pb _{.67} Sr _{.33} (NO ₃) ₂	12m	53	(trigonal) Lithium tungsten oxide hydrate,	1m	25
Lead sulfate (anglesite), PbSO ₄	3	67	Li ₂ WO ₄ ·0.5H ₂ O	2m	20
Lead sulfide (galena), PbS	2	18	Lithium uranium fluoride, LiUF ₅	7m	131
Lead tin oxide, Pb ₂ SnO ₄	10m	29	Lutetium arsenate, LuAsO ₄	5m	36
Lead titanium oxide (macedonite),			Lutetium manganese oxide, LuMnO ₃	2m	23
PbTiO ₃	5	39	Lutetium nitride, LuN	4m	62
Lead tungsten oxide (stolzite), PbWO ₄ (tetragonal)	5m	34	Lutetium oxide, Lu ₂ 0 ₃ Lutetium vanadium oxide, LuVO ₄	1m 5m	27 37
Lead uranium oxide, Pb ₃ UO ₆	8m	109	Magnesium, Mg	1	10
Lithium aluminum fluoride,			Magnesium aluminum oxide (spinel),		
α-Li ₃ AlF ₆	8m	111	MgAl ₂ O ₄	9 m	25
Lithium arsenate, Li ₃ AsO ₄	2m	19	Magnesium aluminum silicate (low		
Lithium azide, LiN ₃	8m	113	cordierite), Mg ₂ Al ₄ Si ₅ O ₁₈	1	20
Lithium barium fluoride, LiBaF ₃ Lithium beryllium fluoride, Li ₂ BeF ₄	5m 7m	35 126	(orthorhombic)	1m	28
Lithium borate, Li ₂ B ₄ O ₇	8m	114	(indialite) Mg ₂ Al ₄ Si ₅ O ₁₈		
Lithium bromide, LiBr	4	30	(hexagonal)	1m	29
Lithium calcium aluminum boron			Magnesium aluminum silicate	,	
hydroxy silicate, liddicoatite,	16-	42	(pyrope), Mg ₃ Al ₂ (SiO ₄) ₂	4m	24
$Ca(Li,Al)_3Al_6B_3Si_6O_{27}(0,OH)_3(OH,F)$ Lithium carbonate, Li_2CO_3	16m 8m	42	Magnesium borate, Mg ₂ B ₂ O ₅ (triclinic)	4m	25
Lithium chlorate hydrate,	Oili	72	Magnesium bromide, MgBr ₂	4m	62
LiClO ₄ ·3H ₂ O	8	34	Magnesium bromide hydrate,		
Lithium chloride, LiCl	1	62	MgBr ₂ ·6H ₂ 0	11m	35
Lithium chromium oxide hydrate,	2.6	, ,	Magnesium carbonate (magnesite),	_	0.0
Li ₂ CrO ₄ ·2H ₂ O	16m	44	MgCO ₃	7	28
Lithium fluoride, LiF Lithium gallium oxide, LiGaO ₂	1 10m	61 31	Magnesium cerium nitrate hydrate, Mg ₃ Ce ₂ (NO ₃) ₁₂ ·24H ₂ O	10	20
Lithium hydroxide hydrate, LiOH·H ₂ O	11m	92	Magnesium chlorate hydrate,	10	20
Lithium iodate, LiIO ₃ (hexagonal)	7	26	$Mg(ClO_4)_2 \cdot 6H_2O \dots$	7m	30
Lithium iodate, LiIO ₃ (tetragonal)	10m	33	Magnesium chloride (chloro-		
Lithium molybdenum oxide, Li ₂ MoO ₄		•	magnesite), MgCl ₂	11m	94
(trigonal)	lm 6m	23	Magnesium chloride hydrate,	7	125
Lithium niobium oxide, LiNbO ₃ Lithium nitrate, LiNO ₃	6m 7	22 27	MgCl ₂ ·12H ₂ O Magnesium chloride hydrate	7m	135
Lithium oxide, Li ₂ 0	lm	25	(bischofite), MgCl ₂ ·6H ₂ O	11m	37
Lithium phosphate hydrate,			Magnesium chromium oxide		
Li ₃ P ₃ O ₉ ·3H ₂ O	2m	20	(magnesiochromite), MgCr ₂ O ₄	9	34

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Magnesium chromium oxide hydrate,			Manganese iron oxide (jacobsite),		
MgCrO ₄ ·5H ₂ O	15m	39	MnFe ₂ O ₄	9	36
Magnesium fluoride (sellaite), MgF ₂ Magnesium fluoride silicate	4	33	Manganese(II) oxide (manganosite), MnO	5	45
(humite), Mg ₇ F ₂ Si ₃ O ₁₂	1m	30	Manganese oxide (pyrolusite), β-MnO ₂	10m	43 39
Magnesium fluoride silicate			Manganese oxide (bixbyite), α-Mn ₂ O ₃	11m	95
(norbergite), $Mg_3F_2SiO_4$	10	39	Manganese oxide (hausmannite),		
Magnesium gallium oxide, MgGa ₂ O ₄	10	36	Mn ₃ 0 ₄	10m	38
Magnesium germanium oxide, Mg ₂ GeO ₄ (cubic)	10	37	Manganese oxide hydroxide, groutite, α -Mn00H	llm	97
Magnesium germanium oxide,	10	31	Manganese phosphate, Mn(PO ₃) ₂	14m	21
Mg ₂ GeO ₄ (orthorhombic)	10	38	Manganese phosphate, Mn ₂ P ₂ O ₇	15m	41
Magnesium hydrogen phosphate			Manganese phosphate, $Mn_3(PO_4)_2$	16m	47
hydrate, newberyite, MgHPO ₄ ·3H ₂ O	7 m	139	Manganese selenide, MnSe	10	41
Magnesium hydroxide (brucite),	6	20	Manganese sulfate hydrate	16-	60
Mg(OH) ₂ Magnesium iron hydroxide carbonate	6	30	(szmikite), MnSO ₄ ·H ₂ O Manganese sulfide (alabandite),	16m	49
hydrate, pyroaurite,			α-MnS	4	11
$Mg_6Fe_2(OH)_{16}CO_3\cdot 4H_2O$ (rhomb.)	10m	104	Manganese titanium oxide		
Magnesium iron hydroxide carbonate			(pyrophanite), MnTiO ₃	15m	42
hydrate, sjögrenite,	10	100	Manganese(II) tungsten oxide	_	0.1
Mg ₆ Fe ₂ (OH) ₁₆ CO ₃ ·4H ₂ O, (hexag.)	10m	103	(huebnerite), MnWO ₄	2m	24 75
Magnesium lanthanum nitrate hydrate, Mg ₃ La ₂ (NO ₃) ₁₂ ·24H ₂ O	lm	22	Manganese vanadium oxide, Mn ₂ V ₂ O ₇ Mercury amide chloride, HgNH ₂ Cl	9m 10m	40
Magnesium manganese oxide, MgMn ₂ O ₄	10m	35	Mercury ammine chloride,	10111	70
Magnesium mercury, MgHg	6m	84	Hg(NH ₃) ₂ Cl ₂	11m	39
Magnesium molybdenum oxide, MgMoO ₄	7m	28	Mercury bromate, Hg(BrO ₃) ₂	10m	107
Magnesium nickel oxide, MgNiO ₂	10m	36	Mercury bromide, HgBr ₂	10m	110
Magnesium oxide (periclase), MgO	1200	37	Mercury bromide, Hg2Br2	7	33
Magnesium phosphate, $Mg(PO_3)_2$ Magnesium phosphate, α - $Mg_2P_2O_7$	13m 9m	26 73	Mercury chloride, HgCl ₂ Mercury chloride (calomel),	13m	29
Magnesium selenide, MgSe	5m	70	Hg ₂ Cl ₂	13m	30
Magnesium selenite hydrate,			Mercury chloride sulfide,		
MgSeO ₃ ·6H ₂ O	8m	116	α -Hg ₃ Cl ₂ S ₂	8m	118
Magnesium silicate, enstatite,			Mercury(II) cyanide, Hg(CN) ₂	6	35
MgSiO ₃	6	32	Mercury(II) fluoride, HgF ₂ Mercury(I) iodide, HgI	2m 4	-25 49
Mg ₂ SiO ₄	1	83	Mercury(II) iodide, HgI ₂ (tetragonal)		32
Magnesium sulfate hydrate	_		Mercury(II) oxide (montroydite),		
(kieserite), MgSO ₄ ·H ₂ O	16m	46	HgO	9	39
Magnesium sulfate hydrate	_		Mercury(II) selenide (tiemannite),	7	0.5
(epsomite), MgSO ₄ ·7H ₂ O	7 7	30	HgSe Mercury sulfate, HgSO ₄	7 16m	35 50
Magnesium sulfide, MgS	′	31	Mercury sulfate, Hg ₂ SO ₄	16m	52
MgSO ₃ ·6H ₂ O	9m	26	Mercury(II) sulfide (cinnabar),		
Magnesium tin, Mg ₂ Sn	5	41	HgS (hexagonal)	4	17
Magnesium tin oxide, Mg ₂ SnO ₄	10m	37	Mercury(II) sulfide (metacinnabar),	,	.07
Magnesium titanium oxide	_	10	HgS (cubic)	4 1	21 20
(geikielite), MgTiO ₃	5 12m	43 25	Molybdenum, Mo	10m	
Magnesium tungsten oxide, MgWO ₄	13m	27	Molybdenum osmium, Mo ₃ Os	6m	115 28 30
Manganese, α-Mn	7m	142	Molybdenum oxide (molybdite), MoO ₃	3	[30
Manganese aluminum oxide (galaxite),			Molybdenum sulfide (molybdenite),		
MnAl ₂ 0 ₄	9	35	MoS ₂	5	130
Manganese bromide, MnBr ₂	4m	63	Neodymium arsenate, NdAsO ₄	4m 4m	12%
Manganese(II) carbonate (rhodochrosite), MnCO ₃	7	32	Neodymium arsenide, NdAs Neodymium borate, NdBO ₃	1m	132
Manganese chloride (scacchite),	,	32	Neodymium chloride, NdCl ₃	1m	1[3]3
MnCl ₂	8m	43	Neodymium chloride oxide, NdOCl	8	်္ဒိ37
Manganese chloride hydrate,			Neodymium fluoride, NdF ₃	8	147 1498 1693 1693 1693 1693 1693 1693 1693 1693
MnCl ₂ ·2H ₂ O	11m	38	Neodymium oxide, Nd ₂ O ₃	4 11m) 26 1) 40
Manganese chloride hydrate,	9m	28	Neodymium phosphate, NdPO ₄ Neodymium selenide, NdSe	11m 5m	971
MnCl ₂ ·4H ₂ O Manganese cobalt oxide, MnCo ₂ O ₄	9m	30	Neodymium silver, NdAg	5m	: ³ 71
Manganese fluoride, MnF ₂	10m	105	Neodymium vanadium oxide, NdVO ₄	4m	30
Manganese iodide, MnI ₂	4m	63	Neptunium nitride, NpN	4m	1064 1013
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Nickel arsenide (rammelsbergite), NiAs ₂	10	42	K ₂ BaNi(NO ₂) ₆ Potassium borate hydroxide hydrate,	9m	32
Nickel arsenic sulfide	10	72	K ₂ B ₄ O ₅ (OH) ₄ ·2H ₂ O	15m	46
(gersdorffite), NiAsS	1m	35	Potassium boron hydride, KBH ₄	9	44
Nickel bromide, NiBr ₂	10m	119	Potassium bromate, KBrO ₃	7	38
Nickel(II) carbonate, NiCO3			Potassium bromide, KBr	1	66
(trigonal)	1m	36	Potassium bromide chloride,		
Nickel chloride, NiCl ₂	9 m	81	KBr _{0.5} Cl _{0.5}	8m	46
Nickel chloride hydrate, NiCl ₂ ·6H ₂ O	11m	42	Potassium bromide iodide, KBr _{.33} 1 _{.67}	11m	44
Nickel fluoride, NiF ₂	10m	121	Potassium bromide iodide,		
Nickel fluoride hydrate, NiF ₂ ·4H ₂ O	11m	43	KBr _{.67} l _{.33}	11m	45
Nickel gallium oxide, NiGa ₂ O ₄	10	45	Potassium cadmium fluoride, KCdF ₃	8m	47
Nickel germanium oxide, Ni ₂ GeO ₄	9	43	Potassium cadmium sulfate,		
Nickel iron oxide (trevorite),			$K_2Cd_2(SO_4)_3$	7m	34
NiFe ₂ O ₄	10	44	Potassium calcium carbonate	0	
Nickel nitrate hydrate,	1.0	26	(fairchildite), K ₂ Ca(CO ₃) ₂	8m	48
Ni(NO ₃) ₂ ·6H ₂ O	12m 1	26 47	Potassium calcium chloride, KCaCl ₃	7m 8m	36 49
Nickel phosphate, Ni(PO ₃) ₂	14m	22	Potassium calcium fluoride, KCaF ₃ Potassium calcium magnesium sulfate		49
Nickel phosphide, Ni ₁₂ P ₅	9m	83	$K_2CaMg(SO_4)_3$, 7m	37
Nickel silicon fluoride hydrate,	J	0,5	Potassium calcium nickel nitrite,	,	3,
NiSiF ₆ ·6H ₂ O	8	38	$K_2CaNi(NO_2)_6$	9m	33
Nickel sulfate, NiSO ₄	2m	26	Potassium calcium sulfate,		
Nickel sulfate hydrate (retgersite),			$K_2Ca_2(SO_4)_3$	7 m	39
NiSO ₄ ·6H ₂ O	7	36	Potassium calcium sulfate hydrate		
Nickel sulfide, millerite, NiS	1m	37	(syngenite), $K_2Ca(SO_4)_2 \cdot H_2O \dots$	14m	25
Nickel tungsten oxide, NiWO ₄	2m	27	Potassium cerium fluoride, β-KCeF ₄	12m	59
Nickel yttrium, Ni ₃ Y	10m	123	Potassium chlorate, KClO ₃	3m	42
Niobium chloride oxide, NbCl ₃ O	7m	148	Potassium chlorate, KClO ₄	6	43
Niobium osmium, Nb ₃ Os	6m	30	Potassium chloride (sylvite), KCl	1	65
Niobium platinum, Nb ₃ Pt	6m	31	Potassium chromium oxide, K ₃ CrO ₈	3m	44
Niobium silicide, NbSi ₂	8	39	Potassium chromium oxide (lopezite)		67
Niobium silicide, α-Nb ₅ Si ₃ Niobium silicide, β-Nb ₅ Si ₃	15m 15m	43 44	$K_2Cr_2O_7$	15m	47
Osmium, Os	4	8	$K_2(CrO_4)_{.33}(SO_4)_{.67}$	12m	28
Osmium titanium, OsTi	6m	85	Potassium chromium oxide sulfate,	± 2	
Palladium, Pd	1	21	$K_2(CrO_4)_{.67}(SO_4)_{.33}$	12m	27
Palladium hydride, PdH _{0.706}	5m	72	Potassium chromium sulfate,		
Palladium oxide, PdO	4	27	$KCr(SO_4)_2$	16m	58
Palladium selenium (palladseite),			Potassium chromium sulfate hydrate,		
Pd ₁₇ Se ₁₅	16m	139	$KCr(SO_4)_2 \cdot 12H_2O \dots$	6	39
Palladium vanadium, PdV ₃	6m	32	Potassium cobalt(ll) fluoride,		
Phosphorus bromide, PBr ₇	7m	150	KCoF ₃	6m	37
Phosphorus oxide (stable form I),	Om.	06	Potassium cobalt fluoride, K ₂ CoF ₄	11m	46
P ₂ O ₅ (orthorhombic) Phosphorus oxide (stable form II),	9m	86	Potassium cobalt nitrite, $K_3Co(NO_2)_6$	9	45
P ₂ O ₅ (orthorhombic)	9m	88	Potassium cobalt(11) sulfate,		73
Phosphorus oxide (metastable form),	,	00	$K_2Co_2(SO_4)_3$	6m	35
P ₄ O ₁₀ (rhombohedral)	9 m	91	Potassium copper chloride, KCuCl ₃	7m	41
Platinum, Pt	1	31	Potassium copper chloride hydrate		
Platinum titanium, PtTi ₃	6m	33	(mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$	9m	34
Platinum vanadium, PtV ₃	6m	34	Potassium copper(ll) fluoride,		
Plutonium arsenide, PuAs	4m	65	KCuF ₃	6m	38
Plutonium phosphide, PuP	4m	65	Potassium cyanate, KCNO	7	39
Plutonium telluride, PuTe	4m	66	Potassium cyanide, KCN	1	77
Potassium aluminum sulfate,	Om	21	Potassium fluoride, KF	1	64
KAl(SO ₄) ₂ Potassium aluminum sulfate hydrate	9m	31	Potassium germanium fluoride, K ₂ GeF ₆	6	41
(potash alum), KA1(SO ₄) ₂ ·12H ₂ O	6	36	Potassium hydrogen arsenate,	Ü	41
Potassium barium chromium oxide,		,,,	KH ₂ AsO ₄	1m	38
$-K_2Ba(CrO_4)_2$	14m	23	Potassium hydrogen phosphate,		
Potassium barium iron titanium			КН ₂ РО ₄	3	69
oxide, K _{1.16} Ba _{0.72} Fe _{0.36} Ti _{5.58} O ₁₃	´16m	147	Potassium hydroxide, KOH at 300 °C	4m	66
Potassium barium molybdenum oxide,			Potassium iodate, KlO ₃	15m	48
$K_2Ba(MoO_4)_2$	14m	24	Potassium iodate, KlO ₄	7	41
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Detection indida VI				Potagojum giligan fluorida		
Potassium iodide, Kl Potassium iron chloride hydrate	1	68		Potassium silicon fluoride (hieratite), K ₂ SiF ₆	5	50
(erythrosiderite), K ₂ FeCl ₅ ·H ₂ O	14m	27		Potassium silver cyanide, KAg(CN) ₂	8m	78
Potassium iron cyanide, K ₃ Fe(CN) ₆	9m	35		Potassium sodium aluminum fluoride	Oili	, 0
Potassium iron(II) fluoride, KFeF ₃	6m	39		(elpasolite), K ₂ NaAlF ₆	9m	43
Potassium iron fluoride, K ₃ FeF ₆	9m	37		Potassium sodium bromide,		
Potassium iron sulfate (yavapaiite),				K.2Na.8Br	12m	62
KFe(SO ₄) ₂	16m	59		Potassium sodium bromide,		
Potassium lead chloride, KPb ₂ Cl ₅	13m	33		K _{.4} Na _{.6} Br	12m	62
Potassium lead chromium oxide,	7.4			Potassium sodium bromide,	7.0	60
$K_2Pb(CrO_4)_2$	14m	28		K ₆ Na ₄ Br	12m	62
Potassium lead molybdenum oxide,	14m	29		Potassium sodium bromide,	12m	62
K ₂ Pb(MoO ₄) ₂ Potassium lead phosphate,	T→III	43		K _{.8} Na _{.2} Br Potassium sodium chloride,	14111	02
$K_2 Pb (PO_3)_4 \dots$	15m	50		K ₂ Na ₈ Cl	12m	63
Potassium lead selenate,				Potassium sodium chloride,		
$K_2Pb(SeO_4)_2$	15m	52		K.4Na.6Cl	12m	63
Potassium lead sulfate (palmierite),				Potassium sodium chloride,		
$K_2Pb(SO_4)_2$	14m	30		K _{.6} Na _{.4} Cl	12m	63
Potassium magnesium chloride				Potassium sodium chloride,	1.0	60
hydrate (carnallite), KMgCl ₃ ·6H ₂ O	8m	50		K 8Na 2Cl	12m	63
Potassium magnesium chromium oxide,	0	E 2		Potassium sodium sulfate,	6m	48
$K_2Mg_2(CrO_4)_3$	8m 6m	52 42		$K_{.67}Na_{1.33}SO_4$	6m	50
Potassium magnesium fluoride, Migra	OIII	44		Potassium sodium sulfate	Oili	50
K_2MgF_4	10m	42		(aphthitalite), K ₃ Na(SO ₄) ₂	6m	52
Potassium magnesium selenate	10			Potassium strontium chromium oxide,		
hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$	10m	43		$K_2Sr(CrO_4)_2$	15m	57
Potassium magnesium sulfate				Potassium strontium selenate,		
(langbeinite), $K_2Mg_2(SO_4)_3$	6m	40		$K_2Sr(SeO_4)_2$	15m	58
Potassium magnesium sulfate hydrate				Potassium strontium sulfate		
(picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$	8m	54		(kalistrontite), K ₂ Sr(SO ₄) ₂	14m	31
Potassium manganese(II) fluoride,	6-	/. E		Potassium sulfate, K ₂ S ₂ O ₇	9m	99 62
KMnF ₃ Potassium manganese oxide, KMnO ₄	6m 7	45 42		Potassium sulfate (arcanite), K ₂ SO ₄ Potassium sulfide, K ₂ S	3 10m	127
Potassium manganese (II) sulfate	,	44		Potassium telluride, K ₂ Te	10m	128
(manganolangbeinite), K ₂ Mn ₂ (SO ₄) ₃	6m	43		Potassium thiocyanate, KCNS	8	44
Potassium molybdenum oxide, K ₂ MoO ₄	15m	53		Potassium tin chloride, K ₂ SnCl ₆	6	38
Potassium molybdenum oxide phos-				Potassium titanium fluoride, K2TiF6	7	40
phate hydrate, K ₃ (MoO ₃) ₁₂ PO ₄ ·4H ₂ O	8	43		Potassium tungsten oxide, K ₂ WO ₄	11m	47
Potassium nickel fluoride, KNiF ₃	7m	42		Potassium vanadium oxide, KV ₃ O ₈	8m	56
Potassium nickel fluoride, K ₂ NiF ₄	10m	45		Potassium zinc bromide hydrate,	7.7	7.0/
Potassium nickel(II) sulfate,	(10		KZnBr ₃ ·2H ₂ O	llm	104
K ₂ Ni ₂ (SO ₄) ₃	6m 8m	46 120		Potassium zinc fluoride, KZnF ₃	5 10m	51 46
Potassium niobium fluoride, K_2NbF_7 Potassium nitrate (niter), KNO_3	3	58		Potassium zinc fluoride, K ₂ ZnF ₄ Potassium zinc iodide hydrate,	10111	40
Potassium nitrite, KNO ₂	9m	38		KZnI ₃ ·2H ₂ O	11m	107
Potassium nitrosyl ruthenium				Potassium zinc sulfate, K ₂ Zn ₂ (SO ₄) ₃	6m	54
chloride, K ₂ NORuCl ₅	16m	61		Potassium zinc sulfate hydrate,		
Potassium oxide, K ₂ O	10m	125		$K_2Zn(SO_4)_2 \cdot 6H_2O \dots$	7m	43
Potassium platinum bromide, K ₂ PtBr ₆	8	40		Potassium zinc vanadium oxide		
Potassium platinum chloride,	1.0	۰,		hydrate, K ₂ Zn ₂ V ₁₀ O ₂₈ ·16H ₂ O	3m	45
K ₂ PtCl ₆	13m	34		Potassium zirconium fluoride,	0	1.6
Potassium platinum fluoride,	6	42		K ₃ ZrF ₇ Praseodymium arsenate, PrAsO ₄	9 4m	46 32
K ₂ PtF ₆ Potassium rhenium chloride, K ₂ ReCl ₆	2m	28		Praseodymium arsenide, PrAs	4m	67
Potassium rhenium oxide, KReO ₄	8	41		Praseodymium chloride, PrCl ₃	1m	39
Potassium rubidium chloride,	, and the second			Praseodymium chloride oxide, PrOCl	9	47
K _{0.5} Rb _{0.5} Cl	8m	76		Praseodymium fluoride, PrF ₃	5	52
Potassium rubidium chromium oxide,				Praseodymium sulfide, PrS	410	67
KRbCrO ₄	12m	29		Praseodymium vanadium oxide, PrVO ₄	5m	40
Potassium ruthenium chloride,	7.0			Praseodymium zinc, PrZn	5m	72
K ₂ RuCl ₆	10	46		Rhenium, Re	2	13 9
Potassium ruthenium oxide chloride	10	47		Rhodium, Rh	3 6m	56
hydrate, $K_4Ru_2OCl_{10} \cdot H_2O$ Potassium selenate, K_2SeO_4	9m	47		Rhodium vanadium, RhV ₃ Rubidium aluminum sulfate	JIII	50
Potassium selenide, K ₂ Se	10m	126		hydrate, RbA1(SO ₄) ₂ ·12H ₂ O	6	44
Potassium selenium bromide, K ₂ SeBr ₆	8	41	174			
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Rubidium amide, RbNH ₂	5m	73	Rubidium selenate, Rb ₂ SeO ₄	9m	44
Rubidium barium chromium oxide, Rb ₂ Ba(CrO ₄) ₂	14m	32	Rubidium silicon fluoride, Rb ₂ SiF ₆ Rubidium strontium chloride,	6	49
Rubidium barium molybdenum oxide,			RbSrCl ₃	7m	54
Rb ₂ Ba(MoO ₄) ₂	15m 8	59 45	Rubidium strontium chromium oxide, $Rb_2Sr(CrO_4)_2$	15m	64
Rubidium bromide, RbBr	7	43	Rubidium strontium sulfate,		
Rubidium cadmium chloride, high form, RbCdCl ₃ (tetragonal)	5m	43	$Rb_2Sr(SO_4)_2$	15m 8	65 48
Rubidium cadmium chloride,	Jiii	43	Rubidium tellurium bromide,	J	40
low form, RbCdCl ₃ (orthorhombic)	5m	41	Rb ₂ TeBr ₆	8	46
Rubidium cadmium sulfate, Rb ₂ Cd ₂ (SO ₄) ₃	7m	45	Rb ₂ TeCl ₆	8	48
Rubidium calcium chloride, RbCaCl ₃	7m	47	Rubidium tin chloride, Rb ₂ SnCl ₆	6	46.
Rubidium calcium fluoride, RbCaF ₃	8m	57	Rubidium zinc fluoride, RbZnF ₃	7m	57
Rubidium calcium sulfate, Rb ₂ Ca ₂ (SO ₄) ₃	7 m	48	Rubidium zinc sulfate hydrate, Rb ₂ Zn(SO ₄) ₂ ·6H ₂ O	7 m	55
Rubidium chlorate, RbClO ₃	8	47	Ruthenium, Ru	4	5
Rubidium chlorate, RbClO ₄	2m	30	Ruthenium titanium, RuTi	6m	86
Rubidium chloride, RbCl	4	41	Samarium arsenate, SmAsO ₄	4m	33
Rubidium chromium oxide, Rb ₂ CrO ₄	3m	46	Samarium arsenide, SmAs	4m	68
Rubidium chromium oxide, Rb ₂ Cr ₂ O ₇	15m	60	Samarium chloride, SmCl ₃	lm lm	40 43
Rubidium chromium sulfate hydrate, RbCr(SO ₄) ₂ ·12H ₂ O	6	47	Samarium chloride oxide, SmOCl Samarium fluoride, SmF ₃	1m	41
Rubidium cobalt(II) chloride,	Ŭ	• •	Samarium oxide, Sm ₂ O ₃ (cubic)	4m	34
RbCoCl ₃	6m	57	Samarium silver, SmAg	5m	73
Rubidium cobalt fluoride, RbCoF ₃	8m	58	Samarium tin oxide, Sm ₂ Sn ₂ O ₇	8m	77
Rubidium cobalt sulfate,	0	5.0	Samarium vanadium oxide, SmVO ₄	5m	47
Rb ₂ Co ₂ (SO ₄) ₃	8m	59	Scandium arsenate, ScAsO ₄	4m	35 68
Rubidium copper chloride hydrate, Rb ₂ CuCl ₄ ·2H ₂ O	10m	47	Scandium arsenide, ScAs Scandium oxide, Sc ₂ O ₃	4m 3	27
Rubidium copper sulfate hydrate,	10111	7,	Scandium phosphate, ScPO ₄	8	50
$Rb_2Cu(SO_4)_2 \cdot 6H_2O$	8m	61	Scandium silicate (thortveitite),		
Rubidium fluoride, RbF	8m	63	Sc ₂ Si ₂ O ₇	7 m	58
Rubidium iodate, RbIO ₃	15m	62	Selenium, Se	_5	54
Rubidium iodate, RbIO ₄	2m 4	31 43	Selenium oxide (selenolite), SeO ₂ Silicon, Si	7m 13m	60 35
Rubidium iron chloride hydrate,	4	45	Silicon, Si (reference standard)	12m	2
Rb ₂ FeCl ₅ ·H ₂ O	14m	33	Silicon nitride, β-Si ₃ N ₄	14m	116
Rubidium iron sulfate hydrate,			Silicon oxide (\alpha or low		
Rb ₂ Fe(SO ₄) ₂ ·6H ₂ O	8m	64	cristobalite), SiO ₂ (tetragonal)	10	48
Rubidium lead chromium oxide, Rb ₂ Pb(CrO ₄) ₂	14m	34	Silicon oxide (α or low cristobalite), SiO ₂ (tetragonal)		
Rubidium lead molybdenum oxide,	- /		(calculated pattern)	15m	180
$Rb_2Pb(MoO_4)_2$	15m	63	Silicon oxide (α or low quartz),		
Rubidium magnesium chromium oxide,	0		SiO ₂ (hexagonal)	3	24
Rb ₂ Mg ₂ (CrO ₄) ₃ Rubidium magnesium chromium oxide	8m	66	Silicon oxide (β or high cristobalite), SiO ₂ (cubic)	1	42
hydrate, Rb ₂ Mg(CrO ₄) ₂ ·6H ₂ O	8m	68	Silver, Ag	1	23
Rubidium magnesium sulfate,			Silver, Ag (reference standard)	8m	2
$Rb_2Mg_2(SO_4)_3$	7 m	50	Silver arsenate, Ag ₃ AsO ₄	5	56
Rubidium magnesium sulfate	0	7.0	Silver arsenic sulfide,	0	306
hydrate, Rb ₂ Mg(SO ₄) ₂ ·6H ₂ O	8m	70	xanthoconite, Ag ₃ AsS ₃	8m 5	126 57
Rubidium manganese(II) fluoride,	5m	44	Silver bromate, AgBrO ₃ Silver bromide (bromargyrite), AgBr		46
Rubidium manganese sulfate,	0		Silver carbonate, Ag ₂ CO ₃	13m	36
\mathbb{R}^{1}	7m	52	Silver chlorate, AgClO ₃	7	44
Rubidium nickel(II) chloride,		r 0	Silver chloride (chlorargyrite),	,	, ,
RbNiCl ₃	6m	58	AgC1	12m	44
Rubidium nickel sulfate, Rb ₂ Ni ₂ (SO ₄) ₃	8m	72	Silver chromium oxide, Ag ₂ CrO ₄ Silver cyanide, AgCN	12m 9m	30 48
ORubidium nickel sulfate hydrate,	Çili	'-	Silver fluoride, AgeR	5m	53
S Rb ₂ Ni(SO ₄) ₂ ·6H ₂ O	8m	74	Silver iodate, AgIO ₄		49
Rubidium nitrate, RbNO ₃ (trigonal)	5m	45	Silver iodide (iodargyrite), AgI		
Rubidium platinum chloride,	c	5.0	(hexagonal)	8	51
Rubidium platinum fluoride, Rb ₂ PtF ₆	5 6	53 48	Silver iodide, γ-AgI (cubic) Silver manganese oxide, AgMnO ₄	9 7m	48 155
+		, 5	175	/ 111	100

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Silver molybdenum oxide, Ag ₂ MoO ₄	7	45	Sodium chromium oxide hydrate,		
Silver nitrate, AgNO ₃	5	59	Na ₂ CrO ₄ ·4H ₂ O	9m	50
Silver nitrite, AgNO ₂	5 1 m	60 45	Sodium chromium oxide hydrate,	7	62
Silver oxide, Ag ₂ O Silver(II) oxide nitrate, Ag ₇ O ₈ NO ₃	1m 4	61	Na ₂ Cr ₂ O ₇ ·2H ₂ O Sodium chromium oxide sulfate,	7 m	62
Silver phosphate, Ag ₃ PO ₄	5	62	$Na_4(CrO_4)(SO_4)$	11m	55
Silver rhenium oxide, AgReO ₄	8	53	Sodium cobalt nitrite, Na ₃ Co(NO ₂) ₆	15m	70
Silver selenate, Ag ₂ SeO ₄	2m	32	Sodium cobalt(II) sulfate hydrate,		63
Silver sodium chloride, Ago. ₅ Na _{0.5} Cl	8m	79	Na ₂ Co(SO ₄) ₂ ·4H ₂ O Sodium cyanate, NaCNO	6m 2m	61 33
Silver sulfate, Ag ₂ SO ₄	13m	37	Sodium cyanide, NaCN (cubic)	1	78
Silver sulfide (acanthite), Ag ₂ S	10	51	Sodium cyanide, NaCN (orthorhombic)		
Silver terbium, AgTb	5m	74	at 6 °C	1	79
Silver thiocyanate, AgCNS	16m	62 74	Sodium fluoride (villiaumite), NaF	1	63
Silver thulium, AgTm	5m 5m	75	Sodium hydrogen carbonate hydrate, trona, Na ₃ H(CO ₃) ₂ ·2H ₂ O	15m	71
Sodium, Na	9m	105	Sodium hydrogen fluoride, NaHF ₂	5	63
Sodium aluminum chloride silicate,			Sodium hydrogen phosphate,		
sodalite, Na ₈ Al ₆ Cl ₂ (SiO ₄) ₆	7m	158	Na ₃ H(PO ₃) ₄	10m	130
Sodium aluminum fluoride (chiolite),	16m	63	Sodium hydrogen silicate hydrate,	7 m	163
Na ₅ Al ₃ F ₁₄ Sodium aluminum sulfate hydrate	10111	0,5	Na ₂ H ₂ SiO ₄ ·4H ₂ O Sodium hydrogen sulfate hydrate,	7 111	105
(soda alum), NaAl(SO ₄) ₂ ·12H ₂ O	15m	68	NaHSO ₄ ·H ₂ O	9m	52
Sodium azide, α -NaN $_3$, at -90 to			Sodium hydroxide, NaOH at 300 °C	4m	69
-100 °C	8m	129	Sodium iodate, NaIO ₃	7	47
Sodium azide, β-NaN ₃ Sodium beryllium calcium aluminum	8m	130	Sodium iodate, NaIO ₄	7 4	48 31
fluoride oxide silicate, meliphanite			Sodium iron fluoride, Na ₃ FeF ₆	9m	54
(Na _{0.63} Ca _{1.37})Be(Al _{0.13} Si _{1.87})	,		Sodium lanthanum fluoride silicate,		
$(F_{0.75}O_{6.25})$	8m	135	$(Na_2La_8)F_2(SiO_4)_6$	7m	64
Sodium beryllium calcium fluoride			Sodium lanthanum molybdenum oxide,	1.0m	4.0
silicate, leucophanite, NaBeCaFSi ₂ O ₆	8m	138	NaLa(MoO ₄) ₂ Sodium magnesium aluminum boron	10m	49
Sodium borate, Na ₂ B ₄ O ₇	16m	64	hydroxide silicate, dravite,		
Sodium borate, Na ₂ B ₈ O ₁₃	7 m	160	NaMg3Al6B3(OH)4Si6O27	3m	47
Sodium borate hydroxide hydrate	1.6		Sodium magnesium carbonate	22.	F.(
(borax), Na ₂ B ₄ O ₅ (OH) ₂ ·8H ₂ O Sodium boron hydride, NaBH ₄	16m 9	66 51	(eitelite), Na ₂ Mg(CO ₃) ₂	11m	56
Sodium bromate, NaBro ₃	5	65	Sodium magnesium sulfate (vanthoffite), Na ₆ Mg(SO ₄) ₄	15m	72
Sodium bromide, NaBr	3	47	Sodium magnesium sulfate hydrate,		
Sodium bromide chloride,			bloedite, Na ₂ Mg(SO ₄) ₂ ·4H ₂ O	6m	63
NaBr _{.33} Cl _{.67}	11m	49	Sodium magnesium sulfate hydrate	1/m	25
Sodium bromide chloride, NaBr _{.67} Cl _{.33}	11m	50	(loeweite), Na ₁₂ Mg ₇ (SO ₄) ₁₃ ·15H ₂ O Sodium manganese(II) fluoride,	14m	35
Sodium calcium aluminum fluoride	11	30	NaMnF ₃	6m	65
hydrate, thomsenolite,			Sodium manganese sulfate hydrate,		
NaCaAlF ₆ ·H ₂ O	8m	132	$Na_{12}Mn_7(SO_4)_{13} \cdot 15H_2O \dots$	14m	37
Sodium calcium carbonate hydrate,	Qm	106	Sodium mercury(II) chloride hydrate	, 6m	66
pirssonite, Na ₂ Ca(CO ₃) ₂ ·2H ₂ O Sodium calcium phosphate, β-NaCaPO ₄	9m 15m	69	NaHgCl ₃ *2H ₂ O	lm	46
Sodium calcium silicate, Na ₂ CaSiO ₄	10m	48	Sodium molybdenum oxide, Na ₂ Mo ₂ O ₇	9 m	110
Sodium calcium sulfate (glauberite),			Sodium neodymium fluoride silicate,		
Na ₂ Ca(SO ₄) ₂	6m	59	$(Na_2Nd_8)F_2(SiO_4)_6$	7m	66
Sodium carbonate hydrate (thermo-	8	54	Sodium nickel(II) sulfate hydrate, Na ₂ Ni(SO ₄) ₂ ·4H ₂ O	6m	68
natrite), Na ₂ CO ₃ ·H ₂ O Sodium carbonate sulfate, Na ₄ CO ₃ SO ₄	11m	51	Sodium nitrate (soda niter), NaNO ₃	6	50
Sodium carbonate sulfate (burkeite),			Sodium nitrite, NaNO ₂	4	62
$Na_6CO_3(SO_4)_2$	11m	52	Sodium oxide, Na ₂ O	10m	134
Sodium carbonate sulfate,	11	E 2	Sodium phosphate, Na ₃ P ₃ O ₉	3m	49
$Na_6CO_3(SO_4)_2$ Sodium carbonate sulfate,	11m	53	Sodium phosphate hydrate, Na ₃ P ₃ O ₉ ·H ₂ O	3m	50
Na ₆ (CO ₃) ₂ SO ₄	11m	54	Sodium phosphate hydrate,	J.,,	
Sodium chlorate, NaClO ₃	3	51	α -Na ₄ P ₄ O ₁₂ ·4H ₂ O (monoclinic)	13m	39
Sodium chlorate, NaClO ₄	7	10	Sodium phosphate hydrate,	2	25
(orthorhombic)	7 2	49 41	β -Na ₄ P ₄ O ₁₂ *4H ₂ O (triclinic) Sodium phosphate hydrate,	2m	35
Sodium chromium oxide, Na ₂ CrO ₄	9 m	48	Na ₆ P ₆ O ₁₈ ·6H ₂ O	5m	54

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Sodium praseodymium fluoride			Strontium silicate, Sr ₃ SiO ₅	13m	44
silicate, (Na ₂ Pr ₈)F ₂ (SiO ₄) ₆	7 m	68	Strontium sulfate (celestite),	13.11	
Sodium selenate, Na ₂ SeO ₄	9m	55	SrSO ₄	2	61
Sodium selenide, Na ₂ Se	10m	135	Strontium sulfide, SrS	7	52
Sodium silicate, α(III), Na ₂ Si ₂ O ₅	8m	141	Strontium telluride, SrTe	4m	69
Sodium silicate, β-Na ₂ Si ₂ O ₅	10m	136	Strontium tin oxide, SrSnO ₃	8m	80
Sodium silicon fluoride	16	(0	Strontium titanium oxíde, SrTiO ₃	3	44
(malladrite), Na ₂ SiF ₆ Sodium sulfate, Na ₂ SO ₄	16m 11m	68 57	Strontium tungsten oxide, $SrWO_4$ Strontium tungsten oxide, Sr_2WO_5	7 12m	53 32
Sodium sulfate (thenardite), Na ₂ SO ₄	2	59	Strontium vanadium oxide, $Sr_3(VO_4)_2$	15m	73
Sodium sulfide, Na ₂ S	10m	140	Strontium zirconium oxide, SrZrO ₃	9	51
Sodium sulfite, Na ₂ SO ₃	3	60	Sulfamic acid, H ₂ NSO ₃ H	7	54
Sodium telluride, Na ₂ Te	10m	141	Sulfur, S (orthorhombic)	9	54
Sodium tin fluoride, NaSn ₂ F ₅	7m	166	Tantalum, Ta	1	29
Sodium titanium oxide, Na ₂ Ti ₃ O ₇	16m	69	Tantalum silicide, TaSi ₂	8	59
Sodium tungsten oxide, Na ₂ WO ₄	1m	47	Tellurium, Te	1	26
Sodium tungsten(VI) oxide hydrate, Na ₂ WO ₄ ·2H ₂ O	2m	33	Tellurium(IV) oxide (paratellurite) TeO ₂ (tetragonal)	, 7	56
Sodium zinc fluoride, NaZnF ₃	6m	74	Tellurium(IV) oxide, paratellurite,	,	50
Sodium zinc sulfate hydrate,	Oill	, ,	TeO ₂ (tetragonal)	10	55
$Na_2Zn(SO_4)_2 \cdot 4H_2O \dots$	6m	72	Tellurium(IV) oxide, tellurite,		
Sodium zirconium fluoride,			TeO ₂ (orthorhombic)	9	57
Na ₇ Zr ₆ F ₃₁	8m	144	Terbium arsenate, TbAsO ₄	3m	54
Strontium aluminum hydroxide,			Terbium arsenide, TbAs	5m	75
Sr ₃ Al ₂ (OH) ₁₂	10m	50	Terbium nitride, TbN	4m	70
Strontium aluminum oxide, Sr ₃ Al ₂ O ₆	10m	52	Terbium phosphide, TbP	5m	76
Strontium arsenate, $Sr_3(AsO_4)_2$ Strontium azide, $Sr(N_3)_2$	2m 8m	36 146	Terbium selenide, TbSe Terbium sulfide, TbS	5m 5m	76 77
Strontium borate, SrB ₂ O ₄	3m	53	Terbium telluride, TbTe	5m	77
Strontium borate, SrB ₄ O ₇	4m	36	Terbium vanadium oxide, TbVO ₄	5m	56
Strontium bromide fluoride, SrBrF	10m	54	Thallium, α-Tl	16m	73
Strontium bromide hydrate,			Thallium aluminum sulfate hydrate,		
SrBr ₂ ·6H ₂ 0	4	60	$T1A1(SO_4)_2 \cdot 12H_2O$	6	53
Strontium carbonate (strontianite),			Thallium(I) arsenate, Tl ₃ AsO ₄	2m	37
SrcO ₃	3	56	Thallium azide, TlN ₃	8m	82
Strontium chloride, SrCl ₂	4	40	Thallium (I) bromate, TlBrO ₃	8 7	60 57
Strontium chloride fluoride, SrClF Strontium chloride hydrate,	10m	55	Thallium bromide, TlBr Thallium cadmium sulfate,	/	37
SrCl ₂ ·2H ₂ O	11m	58	$Tl_2Cd_2(SO_4)_3$	8m	83
Strontium chloride hydrate,			Thallium(I) chlorate, TlClO ₄	2m	38
SrCl ₂ ·6H ₂ O	4	58	Thallium(I) chlorate, TlClO ₃	8	61
Strontium chloride hydroxide			Thallium(I) chloride, TlCl	4	51
phosphate, Sr ₅ Cl _{.65} (OH) _{.35} (PO ₄) ₃	11m	60	Thallium chromium oxide, Tl ₂ CrO ₄	3m	54
Strontium chromium oxide, Sr ₂ CrO ₄	16m	71	Thallium chromium sulfate hydrate,		
Strontium fluoride, SrF ₂	5	67	$T1Cr(SO_4)_2 \cdot 12H_2O$	6	55
Strontium hydroxide, Sr(OH) ₂ Strontium hydroxide hydrate,	13m	41	Thallium cobalt sulfate, $Tl_2Co_2(SO_4)_3$	8m	85
Sr(OH) ₂ ·H ₂ O	13m	42	Thallium cobalt sulfate hydrate,	Oili	0,5
Strontium hydroxide hydrate,			$Tl_2Co(SO_4)_2 \cdot 6H_2O \dots$	7m	70
Sr(OH) ₂ ·8H ₂ O	13m	43	Thallium copper sulfate hydrate,		
Strontium indium hydroxide,			$T1_2Cu(SO_4)_2 \cdot 6H_2O$	7 m	72
$\operatorname{Sr}_{3}\operatorname{In}_{2}(\operatorname{OH})_{12}$	6m	76	Thallium fluoride, TIF	16m	74
Strontium iodide hydrate,			Thallium gallium sulfate hydrate,		
SrI ₂ ·6H ₂ O	8	58	$T1Ga(SO_4)_2 \cdot 12H_2O$	6	57
Strontium manganese oxide, SrMnO ₃ (cubic)	10m	E 6	Thallium(I) iodate, TlIO ₃ Thallium(I) iodide, TlI	8	62
Strontium manganese oxide,	10m	56	(orthorhombic)	4	53
SrMnO ₃ (hexagonal)	10m	58	Thallium iron sulfate hydrate,	7	55
Strontium molybdenum oxide, SrMoO ₄	7	50	$Tl_2Fe(SO_4)_2 \cdot 6H_2O$	8m	87
Strontium nitrate, $Sr(NO_3)_2$	12m	31	Thallium lead sulfate,		
Strontium oxide, Sr0	5	68	$Tl_2Pb(SO_4)_2$	15m	74
Strontium oxide, SrO ₂	6	52	Thallium magnesium chromium oxide,		
Strontium oxide hydrate, Sr0 ₂ ·8H ₂ O	11m	61	Tl ₂ Mg ₂ (CrO ₄) ₃	8m	89
Strontium phosphate, α-Sr ₂ P ₂ O ₇	11m	62 64	Thallium magnesium sulfate hydrate,	7	7/
Strontium phosphate, α -Sr ₃ (PO ₄) ₂ Strontium scandium oxide hydrate,	11m	64	Tl ₂ Mg(SO ₄) ₂ ·6H ₂ O Thallium manganese sulfate,	7 m	74
Sr ₃ Sc ₂ O ₆ ·6H ₂ O	6m	78	$Tl_2Mn_2(SO_4)_3$	7m	76
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Thallium nickel sulfate hydrate, $T1_2Ni(S0_4)_2 \cdot 6H_2O \dots$	7m	78	Yttrium arsenide, YAs	4m 1m	74 51
Thallium(I) nitrate, TlNO ₃	6	58	Yttrium oxide, Y ₂ O ₃	3	28
Thallium oxide (avicennite), Tl ₂ O ₃	16m	77	Yttrium phosphate (xenotime), YPO ₄	8	67
Thallium(III) oxide, Tl ₂ O ₃	2	28	Yttrium sulfide, YS		80
Thallium(I) phosphate, Tl ₃ PO ₄	7	58	Yttrium telluride, YTe	4m	75
Thallium(III) phosphate, T1PO ₄	7	59	Yttrium titanium oxide, Y ₂ TiO ₅		113
Thallium platinum chloride,			Yttrium vanadium oxide, YVO4		59
Tl ₂ PtCl ₆	5	70	Zinc, Zn	1	16
Thallium silicon fluoride, Tl ₂ SiF ₆	6	56	Zinc aluminum oxide (gahnite),		
Thallium strontium sulfate,			ZnAl ₂ 0 ₄	2	38
$Tl_2Sr(SO_4)_2$	15m	75	Zinc ammine bromide, Zn(NH ₃) ₂ Br ₂	11m	68
Thallium(I) sulfate, Tl ₂ SO ₄	6	59	Zinc ammine chloride, $Zn(NH_3)_2Cl_2$	10m	59
Thallium(I) thiocyanate, T1CNS	8	63	Zinc antimony oxide, ZnSb ₂ O ₄	4m	39
Thallium tin chloride, Tl ₂ SnCl ₆	6	54	Zinc borate, $Zn_4B_6O_{13}$	13m	48
Thallium(I) tungsten oxide, Tl ₂ WO ₄	1m	48	Zinc carbonate, smithsonite, ZnCO ₃	8	69
Thallium zinc sulfate hydrate,			Zinc chlorate hydrate,		
$Tl_2Zn(SO_4)_2 \cdot 6H_2O$	7 m	80	$Zn(ClO_4)_2 \cdot 6H_2O$		79
Thorium arsenide, ThAs	4m	70	Zinc chromium oxide, ZnCr ₂ O ₄		59
Thorium oxide (thorianite), ThO ₂	1	57	Zinc cobalt oxide, ZnCo ₂ O ₄		60
Thulium arsenate, TmAsO ₄	3m	56	Zinc cyanide, $Zn(CN)_2$		73
Thulium arsenide, TmAs	4m	71	Zinc fluoride, ZnF ₂		60
Thulium nitride, TmN	4m	71	Zinc fluoride hydrate, ZnF ₂ ·4H ₂ O		69
Thulium oxide, Tm ₂ O ₃	9	58	Zinc germanium oxide, Zn ₂ GeO ₄	10	56
Thulium telluride, TmTe	4m	72	Zinc hydroxide silicate hydrate,	2	62
Thulium vanadium oxide, TmVO ₄	5m	57 12	hemimorphite, Zn ₄ (OH) ₂ Si ₂ O ₇ ·H ₂ O		62 60
Tin, α -Sn (cubic) Tin, β -Sn (tetragonal)	2 1	24	Zinc iodide, ZnI ₂	9	00
Tin arsenide, SnAs	4m	37	Zinc iron oxide (franklinite),	9m	60
	15m	76	$ZnFe_2O_4$		00
Tin arsenide, $Sn_{3.8}As_3$ Tin(II) fluoride, SnF_2	3m	51	ZnMn ₂ 0 ₄		61
Tin hydrogen phosphate, SnHPO ₄	13m	46	Zinc molybdenum oxide, Zn ₂ Mo ₃ O ₈		173
Tin(IV) iodide, SnI ₄	5	71	Zinc nitrate hydrate,	,	1,5
Tin(II) oxide (romarchite), SnO	4	28	α -Zn(NO ₃) ₂ ·6H ₂ O	12m	36
Tin(IV) oxide (cassiterite), SnO ₂	1	54	Zinc oxide (zincite), ZnO		25
Tin sulfide (berndtite), β -SnS ₂	9m	57	Zinc phosphate, α -Zn ₃ (PO ₄) ₂		80
Tin(II) telluride, SnTe	7	61	Zinc phosphate, β -Zn ₃ (PO ₄) ₂		81
Titanium, Ti	3	4	Zinc phosphate, γ -Zn ₃ (PO ₄) ₂		83
Titanium(III) oxide, TiO _{1.515}	9	59	Zinc phosphate hydrate (hopeite),		
Titanium oxide (anatase), TiO ₂	7m	82	$\operatorname{Zn}_3(\operatorname{PO}_4)_2 \cdot 4\operatorname{H}_20 \dots$	16m	85
Titanium oxide, brookite, TiO ₂			Zinc selenide, ZnSe	3	23
(orthorhombic)	3m	57	Zinc silicate (willemite), Zn ₂ SiO ₄	7	62
Titanium oxide (rutile), TiO ₂	7 m	83	Zinc silicon fluoride hydrate,		
Titanium silicide, Ti ₅ Si ₃	8	64	ZnSiF ₆ ·6H ₂ O		70
Titanium sulfide, TiS ₂	4m	72	Zinc sulfate (zinkosite), ZnSO ₄	7	64
Titanium sulfide, Ti ₂ S	8m	149	Zinc sulfate hydrate (goslarite),	0	7.1
Tungsten, W	1	28	ZnSO ₄ ·7H ₂ O	8	71
Tungsten, W (reference standard)	8m	2	Zinc sulfide (wurtzite), α-ZnS	2	1 /
Tungsten sulfide (tungstenite), WS ₂	8 5m	65	(hexagonal)	2	14
Uranium oxide, UO	5m 2	78	Zinc sulfide (sphaelerite), β-ZnS	2	16
Uranium oxide (uraninite), UO ₂	5m	33 78	(cubic)		16 58
Uranium selenide, USe	4m	73	Zinc telluride, ZnTe		62
Vanadium, V	9m	58	Zinc titanium oxide, ZnTiO ₃	_	49
Vanadium(V) oxide (shcherbinaite),	7111	30	Zinc titanium oxide, Zn_2TiO_4		37
V ₂ O ₅	8	66	Zinc tungsten oxide (sanmartinite),		<i>3</i> .
Vanadium sulfide, α-V ₃ S	14m	118	ZnWO ₄		40
Vanadium sulfide, β-V ₃ S	14m	120	Zirconium, α-Zr		11
Ytterbium arsenate, YbAsO ₄	4m	38	Zirconium hydride, ZrH ₂		60
Ytterbium arsenide, YbAs	4m	73	Zirconium iodate, Zr(IO3)4		51
Ytterbium nitride, YbN	4m	74	Zirconium nitride, ZrN		80
Ytterbium oxide, Yb ₂ O ₃	6m	80	Zirconium oxide, ZrO		81
Ytterbium selenide, YbSe	5m	79	Zirconium phosphide, ZrP	4m	75
Ytterbium telluride, YbTe	5m	79	Zirconium silicate, zircon, ZrSiO ₄	4	68
Ytterbium(III) vanadium oxide,			Zirconium sulfate hydrate		
YbV04	5m	58	(zircosulfate), $Zr(SO_4)_2 \cdot 4H_2O \dots$. 7	66
Yttrium arsenate, YAsO ₄	2m	39			
			170		

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CH ₄ N ₂ O	Urea	7	61
CH ₅ NO ₂	Ammonium formate	11m	9
C ₂ Ag ₂ O ₄	Silver oxalate	9m	47
C ₂ FeO ₄ • 2H ₂ O	Iron oxalate hydrate (humboldtine)	10m	24
C ₂ H ₂ CaO ₄	Calcium formate	8	16
C2H2O4 • 2H2O	Oxalic acid hydrate	16m	55
$C_2H_2O_4Pb$	Lead formate	8	30
C ₂ H ₂ O ₄ Sr	Strontium formate	8	55
C ₂ H ₂ O ₄ Sr·2H ₂ O	Strontium formate hydrate (orthorhombic)	8	56
C ₂ H ₃ KO ₄	Potassium formate-formic acid complex	9m	93
$C_2H_3NaO_2 \cdot 3H_2O$	Sodium acetate hydrate	15m	66
$C_2H_4N_2O_2$	Glyoxime	8m	102
C ₂ H ₇ NO ₂	Ammonium acetate	8m	95
C ₂ H ₈ N ₂ O ₄ ·H ₂ O	Ammonium oxalate hydrate (oxammite)	7	5 39
C ₂ K ₂ O ₄ • H ₂ O	Potassium oxalate hydrate Lithium oxalate	9m 10m	34
C ₂ Li ₂ O ₄ C ₂ Na ₂ O ₄	Sodium oxalate	6m	70
C ₂ Na ₂ O ₄ C ₂ O ₄ Rb ₂ ·H ₂ O ₂	Rubidium oxalate perhydrate	9m	102
C ₃ H ₇ NO ₂	L-Alanine	8m	93
C ₃ H ₇ NO ₂ S	L-Cysteine	11m	86
C ₃ H ₁₀ ClN	Trimethylammonium chloride	9m	113
C ₄ H ₄ CaO ₅ ·2H ₂ O	Calcium malate hydrate	10m	76
C ₄ H ₄ KNaO ₆ • 4H ₂ O	Potassium sodium tartrate hydrate	15m	55
C4H4NO8Y•H2O	Ammonium yttrium oxalate hydrate	8m	97
C ₄ H ₄ Na ₂ O ₆ • 2H ₂ O	Sodium D-tartrate hydrate	11m	110
C4H6C0O4 · 4H2O	Cobalt acetate hydrate	12m	19
$C_4H_6NiO_4 \cdot 4H_2O$	Nickel acetate hydrate	13m	31
C ₄ H ₆ O ₆	D-Tartaric acid	7 m	168
$C_4H_7N_3O$	Creatinine	15m	31
$C_4H_8N_8O_8$	α-HMX	11m	100
$C_4H_8N_8O_8$	β-HMX	11m	102
$C_4H_8N_8O_8$	Octahydro-1,3,5,7-tetranitro-		
	1,3,5,7-tetrazocine,alpha-	11m	100
$C_4H_8N_8O_8$	Octahydro-1,3,5,7-tetranitro-		
2 W D	1,3,5,7-tetrazocine,beta-	11m	102
C ₄ H ₂₂ B ₂₀	bis-(o-Dodecacarborane)	6m	7
C ₅ H ₄ N ₄ O ₃	Uric acid, phase 1 (calc. pattern)	8m	154
C ₅ H ₄ N ₄ O ₃ C ₅ H ₇ CuNO ₄ • 2H ₂ O	Uric acid, phase 1 Copper glutamate hydrate	16m 7m	78 110
C ₅ H ₇ NO ₄ Zn • 2H ₂ O	Zinc glutamate hydrate	7 m	170
C ₆ H ₃ N ₃ O ₇	Picric acid	16m	56
C ₆ H ₅ NO ₂	Nicotinic acid	16m	54
C ₆ H ₆ O ₂	γ-Hydroquinone	8m	107
C ₆ H ₈ Cl ₂ N ₄ Zn	Zinc diimidazole chloride	7 m	123
C ₆ H ₈ O ₆	L-Ascorbic acid	8m	99
C ₆ H ₁₂ O ₆	Dextrose	11m	28
C ₆ H ₁₂ O ₆	α-D-Glucose	11m	28
C ₆ H ₁₅ HoO ₁₂ S ₃ ·9H ₂ O	Holmium ethylsulfate hydrate	1m	18
$C_6H_{15}NdO_{12}S_3 \cdot 9H_2O$	Neodymium ethylsulfate hydrate	9	41
C ₇ H ₅ BrO ₂	o-Bromobenzoic acid	16m	22
C ₇ H ₅ ClO ₂	m-Chlorobenzoic acid	16m	30
C ₇ H ₅ FO ₂	p-Fluorobenzoic acid	16m	36
C ₇ H ₉ NO ₂ S	Methyl sulfonanilide	9m	78
C ₇ H ₁₂ O ₄	Pimelic acid	7m	153
C ₈ H ₄ H _{g2} O ₄	Mercury o-phthalate Potassium hydrogen o-phthalate	10m	113
C ₈ H ₅ KO ₄ C ₈ H ₅ O ₄ T1	Thallium hydrogen phthalate	4m 16m	30 75
C ₈ H ₅ O ₄ H C C ₈ H ₇ N ₃ O ₇	2,4,6-Trinitrophenetole	8m	152
C ₈ H ₇ N ₃ O ₇ C ₈ H ₈ O ₃	p-Anisic acid	16m	132
C ₈ H ₉ NO	Acetanilide (calc. pattern)	14m	38
C ₈ H ₉ NO	Acetanilide	16m	7
C ₈ H ₁₁ N ₂ NaO ₃	Sodium barbital	16m	157
C ₈ H ₁₂ N ₂ O ₃	Barbital, form I	15m	126
C ₈ H ₁₂ N ₂ O ₃	Barbital, form II	15m	128

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C ₈ H ₁₂ N ₂ O ₃	Barbital, form IV	15m	130
C ₉ H ₁₄ N ₂ O ₃	Metharbital	15m	177
$C_{10}H_{12}N_2O_3$	Allobarbital	14m	41
$C_{10}H_{16}C1NO$	(-)-Ephedrine hydrochloride	16m	124
$C_{11}H_{16}N_{2}O_{3}$	Vinbarbital, form I	16m	162
C ₁₁ H ₁₈ N ₂ O ₃	Amobarbital, form I	15m	114
C ₁₁ H ₁₈ N ₂ O ₃	Amobarbital, form II	15m	117
C ₁₂ H ₁₀ N ₂	Azobenzene	7m	86
$C_{12}H_{12}N_2O_3$	Phenobarbital, form III	16m	144
C ₁₂ H ₁₆ Cl ₂ CuN ₈	Copper tetrapyrazole chloride	8m	31
C ₁₂ H ₁₆ Cl ₂ N ₈ Ni	Nickel tetrapyrazole chloride	8m	44
C ₁₂ H ₁₆ CuN ₁₀ O ₆	Copper tetraimidazole nitrate	13m	24
C ₁₂ H ₁₆ N ₂	(N,N)-Dimethyltryptamine	14m	109
C ₁₂ H ₁₆ N ₂ O	Bufotenine	15m	133
C ₁₂ H ₁₆ N ₂ O	Psilocin	16m	152
C ₁₂ H ₂₂ O ₁₁	Sucrose	11m	66
C ₁₂ H ₂₆ N ₂ O ₄	Hexamethylenediammonium adipate	7m	121
C ₁₃ H ₂₁ ClN ₂ O ₂	Procaine hydrochloride	16m	149
C ₁₃ H ₂₁ N ₂ O ₄ P	Psilocybin methanolate	16m	154
C ₁₄ H ₁₁ FO	4-Acetyl-2'-fluorodiphenyl	8m	91
C ₁₄ H ₂₀ ClN ₃ S	Methapyrilene hydrochloride	14m	112
C ₁₅ H ₁₂ O ₂	Dibenzoylmethane	7m	115
C ₁₆ H ₁₃ ClN ₂ O	Diazepam	14m	106
C ₁₆ H ₁₃ N	N-Phenyl-2-naphthylamine	6m	29
C ₁₇ H ₁₉ ClN ₂ S	Chlorpromazine	14m	60
$C_{17}H_{20}C1NO_3 \cdot 3H_2O$	Morphine hydrochloride hydrate	16m	133
C ₁₇ H ₂₂ C1NO ₄	L-Cocaine hydrochloride	16m	114
C ₁₇ H ₂₆ ClN	Phencyclidine hydrochloride	16m	141
C ₁₈ H ₂₂ BrNO ₃ ·2H ₂ O	Codeine hydrobromide hydrate	16m	117
	Cadmium hexaimidazole nitrate	8m	23
C ₁₈ H ₂₄ CdN ₁₄ O ₆ C ₁₈ H ₂₄ N ₁₄ NiO ₆	Nickel hexaimidazole nitrate	7m	27
		15m	119
$C_{18}H_{28}N_2O_4S$ $C_{19}H_{22}C1NO_4 \cdot 2H_2O$	(+)-Amphetamine sulfate	15m	136
	Naloxone hydrochloride hydrate	16m	129
C ₁₉ H ₂₅ ClN ₂	Imipramine hydrochloride	16m	92
C ₂₀ H ₂₆ C1NO ₃	Benactyzine hydrochloride	100	92
C ₂₀ H ₃₄	α-Dihydrophyllocladene, hartite	16	100
C II CITNO	(or bombiccite)	16m	122
C ₂₁ H ₂₃ C1FNO ₂	Haloperidol	16m	127
$C_{21}H_{30}O_{2}$	Cannabidiol	16m	111
$C_{22}H_{30}O_4$	Δ ⁹ -Tetrahydrocannabinolic acid B	16m	160
$C_{24}H_{32}N_2O_2Pd$	Palladium bis-(N-isopropyl-3-	_	4//
0 H W	ethylsalicylaldiminate)	7m	144
C ₂₅ H ₁₅ N ₆	N-Methylphenazinium-7,7,8,8-		111
	tetracyanoquinodimethanide	7m	146
$C_{33}H_{40}N_{2}O_{9}$	Reserpine	8m	123

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Acetanilide	C ₈ H ₉ NO (calc. pattern)	14m	38
Acetanilide	C8H9NO	16m	7
4-Acetyl-2'-fluorodiphenyl	$C_{14}H_{11}FO$	8m	91
Alanine, L-	CH ₃ CHNH ₂ CO ₂ H	8m	93
Allobarbital	$C_{10}H_{12}N_{2}O_{3}$	14m	41
Amobarbital, form I	$C_{11}H_{18}N_2O_3$	15m	114
Amobarbital, form II	C ₁₁ H ₁₈ N ₂ O ₃	15m 8m	117 95
Ammonium acetate Ammonium formate	NH ₄ · CH ₃ CO ₂ NH ₄ HCO ₂	11m	9
Ammonium oxalate hydrate (oxammite)	$(NH_4)_2C_2O_4 \cdot H_2O$	7	5
Ammonium yttrium oxalate hydrate	$NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97
Amphetamine sulfate, (+)-	C ₁₈ H ₂₈ N ₂ O ₄ S	15m	119
p-Anisic acid	С ₈ Н ₈ О ₃	16m	11
Ascorbic acid, L-	C ₆ H ₈ O ₆	8m	99
Azobenzene	C ₆ H ₅ NNC ₆ H ₅	7m	86
Barbital, form I	C ₈ H ₁₂ N ₂ O ₃	15m	126
Barbital, form II Barbital, form IV	$C_{8}H_{12}N_{2}O_{3}$ $C_{8}H_{12}N_{2}O_{3}$	15m 15m	128 130
Benactyzine hydrochloride	$C_{20}H_{26}C1NO_3$	16m	92
o-Bromobenzoic acid	C ₇ H ₅ BrO ₂	16m	22
Bufotenine	$C_{12}H_{16}N_2O$	15m	133
Cadmium hexaimidazole nitrate	$Cd(C_3H_4N_2)_6(NO_3)_2$	8m	23
Calcium formate	$Ca(HCO_2)_2$	8	16
Calcium malate hydrate	$Ca(O_2C)_2(CH_2CHOH) \cdot 2H_2O$	10m	76
Cannabidiol	$C_{21}H_{30}O_{2}$	16m	111
m-Chlorobenzoic acid	C ₇ H ₅ ClO ₂	16m	30 60
Chlorpromazine Cobalt acetate hydrate	C ₁₇ H ₁₉ ClN ₂ S Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	14m 12m	60 19
Cocaine hydrochloride, L-	$C_{17}H_{22}C1NO_4$	16m	114
Codeine hydrobromide hydrate	C ₁₈ H ₂₂ BrNO ₃ ·2H ₂ O	16m	117
Copper glutamate hydrate	$Cu(O_2C)_2(H_2NCHCH_2CH_2) \cdot 2H_2O$	7 m	110
Copper tetraimidazole nitrate	$Cu(C_3H_4N_2)_4(NO_3)_2$	13m	24
Copper tetrapyrazole chloride	$Cu(C_3H_4N_2)_4Cl_2$	8m	31
Creatinine	C ₄ H ₇ N ₃ O	15m	31
Cysteine, L-	HSCH ₂ ·CH(NH ₂)·COOH	11m	86
Dextrose Diazepam	C ₆ H ₁₂ O ₆	11m 14m	28 106
Dibenzoylmethane	C ₁₆ H ₁₃ ClN ₂ O (C ₆ H ₅ CO) ₂ CH ₂	7m	115
α-Dihydrophyllocladene, hartite (or	(3611533) 25112	,	110
bombiccite)	C ₂₀ H ₃₄	16m	122
(N,N)-Dimethyltryptamine	$C_{12}H_{16}N_2$	14m	109
bis-(o-Dodecacarborane)	$C_4B_{20}H_{22}$	6m	7
Ephedrine hydrochloride, (-)-	C ₁₀ H ₁₆ ClNO	16m	124
p-Fluorobenzoic acid	C ₇ H ₅ FO ₂	16m	36
Glucose,α-D- Glyoxime	C ₆ H ₁₂ O ₆	11m 8m	28 102
Haloperidol	$H_2C_2(NOH)_2$ $C_2_1H_2_3C1FNO_2$	16m	127
Hexamethylenediammonium adipate	$(CH_2)_4(CO_2H_3N)_2(CH_2)_6$	7m	121
α-HMX	C ₄ H ₈ N ₈ O ₈	11m	100
β-HMX	$C_4H_8N_8O_8$	11m	102
Holmium ethylsulfate hydrate	$Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O$	1m	18
Hydroquinone	γ-HOC ₆ H ₄ OH	8m	107
Imipramine hydrochloride	C ₁₉ H ₂₅ ClN ₂	16m	129
Iron oxalate hydrate (humboldtine) Lead formate	FeC ₂ O ₄ • 2H ₂ O Pb (HCO ₂) ₂	10m 8	24 30
Lithium oxalate	Li ₂ C ₂ O ₄	10m	34
Mercury o-phthalate	$C_6H_4(CO_2H_8)_2$	10m	113
Methapyrilene hydrochloride	C ₁₄ H ₂₀ ClN ₃ S	14m	112
Metharbital	$C_9H_{14}N_2O_3$	15m	177
Methyl sulfonanilide	C ₆ H ₅ NHSO ₂ CH ₃	9m	78
N-Methylphenazinium-7,7,8,8-tetra-	a II N		2.4.4
Cyanoquinodimethanide	C ₂₅ H ₁₅ N ₆	7m	146
Morphine hydrochloride hydrate Naloxone hydrochloride hydrate	$C_{17}H_{20}C1NO_3 \cdot 3H_2O$ $C_{19}H_{22}C1NO_4 \cdot 2H_2O$	16m 16m	133
maronic hydrochroffue hydrate	0191122011104 21120	10111	136

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2-Naphthylamine, N-phenyl-	C ₁₀ H ₇ NHC ₆ H ₅	6m	29
Neodymium ethylsulfate hydrate	Nd[(C ₂ H ₅)SO ₄] ₃ ·9H ₂ O	9	41
Nickel acetate hydrate	Ni(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	13m	31
Nickel hexaimidazole nitrate	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m	27
Nickel tetrapyrazole chloride	$Ni(C_3H_4N_2)_4Cl_2$	8m	44
Nicotinic acid	C ₆ H ₅ NO ₂	16m	54
Octahydro-1,3,5,7-tetranitro-	952	20	
1,3,5,7-tetrazocine (α-HMX)	C ₄ H ₈ N ₈ O ₈	11m	100
Octahydro-1,3,5,7-tetranitro-	-488-8		100
1,3,5,7-tetrazocine (β-HMX)	C ₄ H ₈ N ₈ O ₈	11m	102
Oxalic acid hydrate	C ₂ H ₂ O ₄ ·2H ₂ O	16m	55
Palladium bis-(N-isopropyl-3-	• Z Z. • 4 2 Z. •	1011	33
ethylsalicylaldiminate)	Pd(C ₁₂ H ₁₆ NO) ₂	7m	144
Phencyclidine hydrochloride	C ₁₇ H ₂₆ ClN	16m	141
Phenobarbital, form III	C ₁₂ H ₁₂ N ₂ O ₃	16m	144
Picric acid	C ₆ H ₃ N ₃ O ₇	16m	56
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m	153
		9m	93
Potassium formate-formic acid complex	KO ₂ CH·HO ₂ CH	4m	30
Potassium hydrogen o-phthalate	C ₆ H ₄ (COOH)(COOK)	9m	39
Potassium oxalate hydrate	K ₂ C ₂ O ₄ · H ₂ O	9m	96
Potassium oxalate perhydrate Potassium sodium tartrate hydrate	K ₂ C ₂ O ₄ ·H ₂ O ₂ C ₄ H ₄ KNaO ₆ ·4H ₂ O	15m	55
· · · · · · · · · · · · · · · · · · ·		16m	149
Procaine hydrochloride Psilocin	C ₁₃ H ₂₁ ClN ₂ O ₂	16m	152
	$C_{12}H_{16}N_{2}O$	16m	154
Psilocybin methanolate	C ₁₃ H ₂₁ N ₂ O ₄ P		123
Reservine	C ₃₃ H ₄₀ N ₂ O ₉	8m	
Rubidium oxalate perhydrate	Rb ₂ C ₂ O ₄ • H ₂ O ₂	9m	102
Silver oxalate	Ag ₂ C ₂ O ₄	9m	47
Sodium acetate hydrate	$C_2H_3NaO_2 \cdot 3H_2O$	15m	66
Sodium barbital	C ₈ H ₁₁ N ₂ NaO ₃	16m	157
Sodium D-tartrate hydrate	(CHOH-CO ₂ Na) ₂ ·2H ₂ O	11m	110
Sodium oxalate	Na ₂ C ₂ O ₄	6m	70
Strontium formate	Sr(CHO ₂) ₂	8	55
Strontium formate hydrate	$Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8	56
Sucrose	C ₁₂ H ₂₂ O ₁₁	11m	66
Tartaric acid, D-	(CHOHCO ₂ H) ₂	7m	168
Δ9-Tetrahydrocannabinolic acid B	C ₂₂ H ₃₀ O ₄	16m	160
Thallium hydrogen phthalate	C ₈ H ₅ O ₄ T1	16m	75
Trimethylammonium chloride	(CH ₃) ₃ NHC1	9m	113
2,4,6-Trinitrophenetole	$C_2H_5OC_6H_2(NO_2)_3$	8m	152
Urea	$CO(NH_2)_2$	7	61
Uric acid, phase l, (calc. pattern)	$C_5H_4N_4O_3$	8m	154
Uric acid (phase 1)	$C_5H_4N_4O_3$	16m	78
Vinbarbital, form I	$C_{11}H_{16}N_{2}O_{3}$	16m	162
Zinc diimidazole chloride	$Zn(C_3H_4N_2)_2Cl_2$	7m	123
Zinc glutamate hydrate	Zn(O ₂ CCHNH ₂ CH ₂ CH ₂ CO ₂)·2H ₂ O	7m	170

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Acanthite, Ag ₂ S	10	51	Clinobisvanite, BiVO ₄	3m	14
Aeschynite CeNbTiO ₆	3m	24	Copper, Cu	1	15
Alabandite, MnS	4	11	Cordierite, Mg ₂ Al ₄ Si ₅ O ₁₈	lm	28
Anatase, TiO ₂	7m	82	Corundum, Al ₂ O ₃	9	3
Andradite, Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22	Cotunnite, PbCl ₂	12m	23
Anglesite, PbSO ₄	3	67	Covellite, CuS	4	13
Anhydrite, CaSO ₄	4	65	Cristobalite (α or low) SiO ₂		
Antarcticite, CaCl ₂ ·6H ₂ O	12m	16	(tetragonal)	10	48
Antimony, Sb	3	14	Cristobalite (α or low) SiO ₂	3.5	300
Aphthitalite, $K_3Na(SO_4)_2$	6m	52	(tetragonal, calculated pattern)	15m	180
Aragonite, CaCO ₃	3	53	Cristobalite (β or high) SiO ₂ (cubic)	1	42
Aragonite, CaCO ₃ (calculated pattern	1) 14m 3	44 62	Cryolithionite, $\text{Li}_3\text{Na}_3\text{Al}_2\text{F}_{12}$ Cryptohalite, $(\text{NH}_4)_2\text{SiF}_6$	9m 5	23 5
Arcanite, K ₂ SO ₄	3	6	Cuprite, Cu ₂ O	2	23
Arsenolite, As ₂ 0 ₃	1	51	*Derbylite, SbFe ₄ Ti ₃ O ₁₃ (OH)	16m	89
Aurostibite, AuSb ₂	7	18	*Diamond, C	2	5
Avicennite, Tl ₂ O ₃	16m	77	*Diaspore, Al ₂ O ₃ ·H ₂ O	3	41
*Azurite, Cu ₃ (OH) ₂ (CO ₃) ₂	10	30	Diopside, CaMg(SiO ₃) ₂	5m	17
*Bahianite, Al _{5.66} Fe _{0.09} Sb _{2.95} O ₁₆ .	16m	87	* Dravite, NaMg ₃ Al ₆ B ₃ Si ₆ O ₂₇ (OH) ₄	3m	47
Baryte, BaSO ₄	10m	12	Eitelite, $Na_2Mg(CO_3)_2$	11m	56
Berlinite, AlPO ₄	10	3	Elpasolite, K ₂ NaAlF ₆	9m	43
Berndtite, SnS ₂	9m	57	<pre>*Enstatite, MgSiO₃</pre>	6	32
*Beryl, Be ₃ Al ₂ Si ₆ O ₁₈	9	13	Epsomite, MgSO ₄ ·7H ₂ O	7	30
Bischofite, MgCl ₂ ·6H ₂ O	11m	37	Erythrosiderite, K ₂ FeCl ₅ ·H ₂ O	14m	27
Bismite, α-Bi ₂ O ₃	3m	17	Eskolaite, Cr ₂ O ₃	5	22
Bismoclite, BiOCl	4	54	Ettringite, Ca ₆ Al ₂ S ₃ O ₁₈ ·3lH ₂ O	8	3
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Bismuthinite, Bi_2S_3	5m 11m	95	Fluorapatite, Ca ₅ F(PO ₄) ₃ Fluorite, CaF ₂	3m 1	69
*Bloedite, Na ₂ Mg(SO ₄) ₂ ·4H ₂ O	6m	63	Forsterite, Mg ₂ SiO ₄	î	83
Boehmite, Al ₂ O ₃ ·H ₂ O	3	38	Franklinite, ZnFe ₂ O ₄	9m	60
*Bombiccite, C ₂₀ H ₃₄	16m	122	Fresnoite, Ba ₂ TiSi ₂ O ₈	9m	14
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*Butlerite, Fe(OH)SO ₄ ·2H ₂ O	10m	95	Goslarite, ZnSO ₄ ·7H ₂ O	8 4	15
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Calomel, Hg ₂ Cl ₂	13m	30	Halite, NaCl	2	41
Carnallite, KMgCl ₃ ·6H ₂ O	8m	50	*Hartite, C ₂₀ H ₃₄	16m	122
Carobbiite, KF	1	64	Hausmannite, Mn_3O_4	10m	38
Cassiterite, SnO ₂	1	54	*Hemimorphite, Zn ₄ (OH) ₂ Si ₂ O ₇ ·H ₂ O	2	62
Celestite, SrSO ₄	2	61	Hetaerolite, ZnMn ₂ O ₄	10m	61
Cerianite, CeO ₂	1	56	*Hexahydroborite, $Ca[B(OH)_4]_2 \cdot 2H_2O$	16m	104
Cerussite, PbCO ₃	2	56	Hieratite, K ₂ SiF ₆	5	50
Cervantite, Sb ₂ O ₄	10	8	Hopeite, $Zn_3(PO_4)_2 \cdot 4H_2O$	16m	85
Chalcokyanite, CuSO ₄	3m	29	Huebnerite, MnWO ₄	2m	24
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Chiolite, Na ₅ Al ₃ F ₁₄	16m	63	Humite, Mg ₇ F ₂ Si ₃ O ₁₂	lm llm	30 18
Chlorargyrite AgCl	7 4	3	Hydrophilite, CaCl ₂	11m 15m	34
Chlorargyrite, AgCl	11m	44 94	Indialite, Mg ₂ Al ₄ Si ₅ O ₁₈	15m	29
Chromatite, CaCrO ₄	7	13	Iodargyrite, AgI	8	51
Chrysoberyl, BeAl ₂ O ₄	- 9	10	Iron, α-Fe	4	3
Cinnabar, HgS	4	17	Jacobsite, MnFe ₂ O ₄	9	36
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Clausthalite, PbSe	5	38	$Ca_2Fe_3Si_3O_{10}(OH,O)_2(OH)_2$	10m	72
÷			Kalistrontite, K ₂ Sr(SO ₄) ₂	14m	31

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Kremersite, (NH ₄ KN ₂ CGL) ₃ -H ₂ O 14m 8 Potash alum, KAl(SG ₃) ₂ :12H ₂ O 6 6 22 Laufastine, CA(IO ₂) ₂ 14m 12 Pyrangyrite, Ag ₃ SbS ₃ 5m 51 12m, Ag ₂ CG ₃ CO ₂ Dalla, CA(IO ₂) ₂ 14m 12 Pyrangyrite, Ag ₃ SbS ₃ 5m 52 23 24 24 24 24 24 24 2			Page			Page
Kremersite, (NH ₄ KN ₂ CGL) ₃ -H ₂ O 14m 8 Potash alum, KAl(SG ₃) ₂ :12H ₂ O 6 6 22 Laufastine, CA(IO ₂) ₂ 14m 12 Pyrangyrite, Ag ₃ SbS ₃ 5m 51 12m, Ag ₂ CG ₃ CO ₂ Dalla, CA(IO ₂) ₂ 14m 12 Pyrangyrite, Ag ₃ SbS ₃ 5m 52 23 24 24 24 24 24 24 2	Kieserite, MgSO. HoO	1.6m	46	Portlandite, Ca(OH)	1	5.8
Laudariet, Cal(Da)2						
Lautarite, Ca(TO ₂)2	Langbeinite, $K_2Mg_2(SO_4)_3$					
Lead, Ph		14m	12		5m	51
### Spring	Lead, Pb	1		Pyrite, FeS ₂	5	29
(0,00)3(0H,F)		8m	138			
Lime, CaO (calculated pattern) 14m 49		1.6	10			
Lime, CaO (calculated pattern) 14m 49						
*Lintarge, PhO (red) 16m 34 Rammelshergite, NiAs2 10 42 Litharge, PhO (red) 2 30 Retgersite, NiSO ₄ (Rip.0 7 32 Altihophosphate, LigPO ₄ 4m 21 Rhodochrosite, MnCO ₃ 7 32 Loeweite, Na12Ngr(SO ₄)1a; UspO ₄ 4m 21 Rhodochrosite, MnCO ₃ 7 32 Loeweite, Na12Ngr(SO ₄)1a; UspO ₄ 4m 35 *Rhoscherite, SnO 4 28 Loeweite, Na12Ngr(SO ₄)1a; UspO ₄ 4m 35 *Rhoscherite, SnO 4m 2m 2m 2m 2m 2m 2m 2m						
Lithinghosphate, LigPO ₃ 4m 21 Rhodorhosite, MinOo ₃ 7 36 Loevlite, Map; PeAs ₂ 10 34 Robarthosite, MinOo ₃ 7 32 Loevlingite, FeAs ₂ 10 34 Robarthosite, MinOo ₃ 7 32 Loevlite, KgCr ₂ O ₇ 15m 35 *Rosenerite, Monoclinic), Be ₂ Ca Lopezite, KgCr ₂ O ₇ 15m 47 (Fe ₂ M ₂ -r) ₂ Al. ₆ r(FO ₄) ₃ : 2H ₂ O ₆ 0 16m 96 **Loeveringite, Ca. ₇ zRK, 33(Y,Th, U, PD), ogTi ₁₂ , 48Fe ₃ , 38Cr ₂ , 28He, 92 **TosAl. ₃ Si ₂ , 2Hn ₀ O ₄ O ₃ as 16m 106 (FO ₄)(610H)·6He) 12m 27 m 83 **Magnesiothomite, MgCr ₂ O ₄ 9 34 Safflorite, CoFeAs ₄ 10 **Magnesiothomite, MgCr ₂ O ₃ 7 28 **Magnesite, MgCO ₃ 7 28 **Magnesite, MgCO ₃ 7 28 **Salammoniac, NH ₂ Cl 1 1 59 **Magnesite, NgCO ₃ 10 31 Sanbartinite, ZhhOq 2m 40 **Maladrite, Nu ₂ O(H ₂ CO ₃ 10 31 Sanbartinite, ZhhOq 2m 40 **Manganolampeinite, KgMn ₂ (SO ₄) ₃ 6m 43 **Scheelite, CabOq 6 23 **Manganolampeinite, KgMn ₂ (SO ₄) ₃ 6m 43 **Scheelite, CabOq 6 23 **Manganolampeinite, KgMn ₂ (SO ₄) ₃ 6m 43 **Scheelite, CabOq 6 23 **Manganolampeinite, NgMn ₂ (SO ₄) ₃ 9 8 Sclenbire, ScO ₂ 7m 60 **Massicot, PbO (yellow) 2 2 32 Scllaite, MgF ₂ 4 33 **Matlockite, PbFCl 1 13m 25 Senarmontite, NgF ₂ O ₃ 3 31 **Matlockite, PbFCl 2 1 3m 25 Senarmontite, Ng ₂ Ce ₂ O ₃ 15m 32 **Melanterite, PeAc ₄ **H ₂ O ₅ 8 8 64 **Marganite, (Ri ₂ All ₄ O ₃ O ₃ 9 9 8 Sclenbire, ReO ₂ 1 5m 32 **Melanterite, ReO ₄ **H ₂ O ₅ 8 8 38 **Silver, Ag (Teference standard) 8 8 2 **Melanterite, ReO ₄ **H ₂ O ₅ 8 8 38 **Silver, Ag (Teference standard) 8 8 2 **Margarite, ReO ₄ **H ₂ O ₅ 9 9 7 8 Scherbinaite, V ₂ O ₅ 8 6 **Melarpenite, ReO ₄ **H ₂ O ₅ 9 9 7 8 Scherbinaite, Ng ₂ Fe ₂ O ₃ 0(Dh) ₁ -4H ₂ O 10m 103 **Melanterite, ReO ₄ **H ₂ O ₅ 9 9 7 9 7 8 Scherbinaite, Ng ₂ Fe ₂ O ₃ 9 9 1 22 **Melanterite, ReO ₄ **H ₂ O ₅ 9 9 7 9 7 8 Scherbinaite, Ng ₂ Fe ₂ O ₃ 9 9 8 12 **Melanterite, ReO ₄ **H ₂ O ₅ 9 9 7 9 7 8 Scherbinaite, Ng ₂ Fe ₂ O ₃ 9 9 9 7 9 9 7 8 Scherbinaite, Ng ₂ Fe ₂ O ₃ 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9						
Lithiophosphate, LigROQ						
Localingite, FeAs2						
Loeweite, Naj,2Mgr,(SO ₂)3,15Hg.0		10	34		4	28
Lopezite, K2Cr2O7	Loeweite, Na ₁₂ Mg ₇ (SO ₄) ₁₃ ·15H ₂ O	14m	35			
Pb)_osTi2_4sFe3_scT2_2sM8_s2	Lopezite, K ₂ Cr ₂ O ₇	15m	47		16m	96
Zr _sall_sgV _slMn_osQ_ss						
Macedonite, PbTi03		1.6	7.07			100
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				Sodalite, Na ₈ Si ₆ Al ₆ O ₂₄ Cl ₂		
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Oldhamite, CaS						
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*Pirssonite, Na ₂ Ca(CO ₃) ₂ ·2H ₂ O 9m 106 Tin, α-Sn (cubic)		_				
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NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

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